

# Orbit spaces of reflection groups with 2, 3 and 4 basic polynomial invariants\*

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## Abstract

Functions which are covariant or invariant under the transformations of a compact linear group can be advantageously expressed in terms of functions defined in the orbit space of the group, i.e. as functions of a finite set of basic invariant polynomials. The equalities and inequalities defining the orbit spaces of all finite coregular real linear groups (most of which are crystallographic groups) with at most four independent basic invariants are determined. For each group  $G$  acting in the Euclidean space  $\mathbb{R}^n$ , the results are obtained through the computation of a metric matrix  $\hat{P}(p)$ , which is defined only in terms of the scalar products between the gradients of a set of basic polynomial invariants  $p_1(x), \dots, p_q(x)$ ,  $x \in \mathbb{R}^n$  of  $G$ ; the semi-positivity conditions  $\hat{P}(p) \geq 0$  are known to determine all the equalities and inequalities defining the orbit space  $\mathbb{R}^n/G$  of  $G$  as a semi-algebraic variety in the space  $\mathbb{R}^q$  spanned by the variables  $p_1, \dots, p_q$ . In a recent paper, the  $\hat{P}$ -matrices, for  $q \leq 4$ , have been determined in an alternative way, as solutions of a universal differential equation; the present paper yields a partial, but significant, check on the correctness and completeness of these solutions. Our results can be easily exploited, in many physical contexts where the study of covariant or invariant functions is important, for instance in the determination of patterns of spontaneous symmetry breaking, in the analysis of phase spaces and structural phase transitions (Landau's theory), in covariant bifurcation theory, in crystal field theory and in most areas of solid state theory where use is made of symmetry adapted functions.

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## 1 Introduction

Functions which are covariant or invariant under the transformations of a compact linear group (hereafter abbreviated in CLG)  $G$  play an important role in physics, and the determination of their properties is often a basic problem to solve.

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An example, which is relevant both to elementary particle and solid state physics, is offered by the determination of the possible patterns of spontaneous symmetry breaking in theories in which the ground state of the system is determined by the minimum of an invariant potential  $V(x)$ .

Let us sketch the relevant physical context. The symmetry group  $G$  of the formalism used to describe a physical system acts as a permutation group on the set of the solutions of the evolution equations. When the ground state of the system is invariant only with respect to a proper subgroup  $G_0 \subset G$ , the  $G$ -symmetry is said to be *spontaneously broken* (see, for instance [1, 2, 3, 4] and references therein) and  $G_0$  turns out to be the *true* symmetry group of the system [5].

One of the most common classical mechanisms of spontaneous symmetry breaking can be formalized in the following way. The ground state is represented by a vector  $x_0$  belonging to the Euclidean space  $\mathbb{R}^n$ , on which  $G$  acts as a group of linear transformations;  $x_0$  is determined as the point at which a  $G$ -invariant potential  $V(x)$  assumes its absolute minimum ( $V$  might be a Higgs potential in a gauge field theory or a thermodynamic potential in a Landau theory of structural phase transitions), and  $G_0$  is the isotropy subgroup of  $G$  at  $x_0$  (the little group of  $G_0$ ). Generally, the potential depends also on parameters  $\gamma$  (for instance scalar self-couplings in Higgs potentials, or pressure and temperature in thermodynamic potentials), that cannot be determined from invariance requirements under transformations of  $G$ . In this case  $x_0$  and  $G_0$  can depend on the  $\gamma$ 's, and various patterns of spontaneous symmetry breaking are allowed, corresponding to distinct structural *phases* of the system.

In supersymmetric field theories the absolute minimum of the potential controls both the spontaneous symmetry and supersymmetry breaking (see, for instance [6] and references therein), and often the features of the two breaking schemes are related [7].

In all the cases just mentioned, the determination of the ground state of the system rests on a precise determination of the point  $x_0$ , where the potential takes on its absolute minimum, and the determination has to be analytical, since the isotropy subgroups of  $G$  at nearby points may be different.

Even if trivial in principle, the analytical determination of the minimum of an invariant potential is generally a difficult computational task (even if one uses polynomial approximations for the potential), owing to the large number  $n$  of the variables  $x_i$  which are often involved. An additional difficulty is related to the degeneracy of the stationary points of the potential, which is an unavoidable consequence of the invariance properties of the potential; it prevents, in fact, a direct application [8] of Morse's theory [9]. Also the use of an extended Morse theory [10] seems not to give big advantages [11].

In 1971, Gufan [12, 13] proposed a new, more economical, approach to the problem, which was based on the remark that a  $G$ -invariant function  $V(x)$  can be expressed as a function  $\hat{V}(p_1, \dots, p_q)$  of a finite set  $p(x) = (p_1(x), \dots, p_q(x))$  of basic polynomial invariants. When the point  $p \in \mathbb{R}^q$  ranges in the domain spanned by  $p(x)$ ,  $x \in \mathbb{R}^n$ , the function  $\hat{V}(p)$  has the same range as  $V(x)$ , but is not plagued by the same degeneracies. Gufan's proposal found immediate applications in crystal field theory (see refs. [14, 15, 16, 17, 18, 19], to cite but a few of the pioneering papers on the subject). A full and correct exploitation of his idea required, however, an exact determination of the ranges of the functions  $p_i(x)$ , a non

trivial problem that was solved only ten years later, when it was independently remarked [20] that any  $G$ -invariant function, being a constant along each orbit of  $G$ , can be considered a function in the orbit space  $\mathbb{R}^n/G$  of the action of  $G$  in  $\mathbb{R}^n$ . As a consequence, the problem of determining the stationary points of  $V(x)$  could be more economically reformulated in  $\mathbb{R}^n/G$  [21], where the  $p_i$ 's can be used advantageously to parametrize the orbits. In  $\mathbb{R}^n/G$ , the images of all the points of  $\mathbb{R}^n$  with the same invariance properties under  $G$  transformations form smooth sub-manifolds, which are usually called *strata*. By varying the parameters  $\gamma$ , the location of the minimum of  $V(x; \gamma)$  may shift to a different stratum, thus causing a (structural) phase transition of the system.

A sensible progress in the characterization of the geometry of the orbit spaces of the CLG's was achieved using the powerful tools of geometric invariant theory [22, 23], which led to the discovery of a simple recipe allowing to build a concrete image of the orbit space of any linear CLG and its stratification [20, 21, 24, 25]. It was shown that the orbit spaces of the CLG's are connected semi-algebraic varieties, whose defining equations and inequalities can be expressed in the form of positivity conditions of matrices  $\hat{P}(p)$  built only in terms of the gradients of the basic polynomial invariants  $p_1(x), \dots, p_q(x)$ :

$$\hat{P}_{ab}(p(x)) = \sum_i^n \frac{\partial p_a(x)}{\partial x_i} \frac{\partial p_b(x)}{\partial x_i}, \quad a, b = 1, \dots, q. \quad (1)$$

Using this result, one can obtain, for instance, a concrete realization of the orbit space of any *coregular*<sup>1</sup> finite linear group. In fact, the class of these groups has been shown to coincide with the class formed by the finite groups generated by reflections (which are almost all crystallographic groups) and explicit or algorithmic descriptions of their basic polynomial invariants have been given by many authors (see for instance [26, 27, 28, 29, 30, 31, 32]).

For a general CLG, the matter is not that simple, since the determination of a minimal complete set of basic invariant polynomials, i.e. of a minimal integrity basis of the ring of polynomial invariants of  $G$ , may be a difficult problem to solve.<sup>2</sup> This serious handicap in the direct approach to the determination of the  $\hat{P}$ -matrix associated to a general CLG stimulated the research, and led to the discovery, of an alternative indirect method of computation of the  $\hat{P}$ -matrices associated to CLG's. These matrices have been shown [36, 37, 38] to be solutions of a *master* differential equation, satisfying convenient initial conditions (*allowable solutions*). The master equation assumes a particularly simple canonical form (*canonical equation*) for compact coregular linear groups (hereafter abbreviated in CCLG's). The form of the canonical equation is the same for all CCLG's; it does involve only the degrees of the elements of the integrity bases as free parameters.

The master equation approach to the determination and classification of the  $\hat{P}$ -matrices gives a strong support to the conjecture that the orbit spaces of all the compact linear groups possessing a basis of  $q$  independent basic polynomial invariants with the same degrees can

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<sup>1</sup> $G$  is said to be coregular if there is no algebraic relation among the elements of a minimal set of its basic invariant polynomials, i.e., among the elements of the minimal integrity bases of the ring of its polynomial invariants.

<sup>2</sup>A complete classification of compact coregular linear groups is known, at present, only for finite groups and for simple [33] and semisimple [34] Lie groups.

be classified in a finite (and small, for small dimensions and degrees) number of isomorphism classes. The conjecture has been proved to hold true for  $q \leq 4$ .

This fact makes the orbit space approach to the study of covariant functions, and in particular of spontaneous symmetry breaking, particularly appealing. In fact, invariance properties are often the only bounds which are imposed on the potential (beyond regularity and stability properties and/or bounds on the degree, when the potential is a polynomial function). If the symmetry groups of the potentials of different theories share isomorphic orbit spaces, the potentials have the same formal expression and the same domain when written as functions in orbit space, despite the completely different physical meaning of the variables and parameters involved in the definition of the potentials. Thus, the problems of determining the geometric features of the phase space, the location and stability properties of the minima of the potential, the number of primary strata (and, consequently, the maximum number of phases) and the allowed transitions between primary strata are identical in all these theories [21, 35, 36, 37].

The pursuit of the ambitious program of determining the orbit spaces of all the CLG's, following the master equation approach, has already given encouraging results, but has left some serious open problems [38]. The main ones are listed below; some of them will be dealt with and partially solved in this paper:

1. All the allowable solutions of the canonical equation have been determined for  $q \leq 4$  (see refs. [37, 39] hereafter referred to as I and II), while for  $q > 4$ , the determination of all the allowable solutions appears to be still possible, but extremely lengthy. The set-up of an inductive procedure for the determination of at least a part of the allowable solutions of the canonical equation is in progress [40, 41].
2. The canonical equation and the associated initial conditions are only a set of necessary conditions that the  $\hat{P}$ -matrices of the CLG's must satisfy; even if quite stringent, they need not be sufficient. Therefore, once the allowable solutions of the canonical equation have been determined, the problem remains of selecting those which are really generated by a group. In this paper we shall give a partial answer to this problem in the case of coregular groups with  $q \leq 4$ .
3. An effective formalization of the condition that there is no algebraic relation among the elements of a minimal integrity basis (minimality + regularity condition) has not yet been found, nor used, in I and II. Thus, it cannot be excluded that some of the allowable  $\hat{P}$ -matrices determined in I and II are indeed associated to non minimal bases or to non-coregular groups.
4. A sound analysis of the structure of the master equation in the general non-coregular case is still missing; some results have been obtained only for non-coregular CLG's with a sole independent relation among the elements of the minimal integrity bases [42].

The paper will be organized in the following way. We shall begin, in §2, with a short survey of the geometry of linear group actions, of the properties of the canonical equation, and we

shall briefly argue on the possibility of classifying the orbit spaces of the CCLG's through the determination of the allowable solutions of the canonical equation. In §3 and §4 we shall determine explicitly the  $\hat{P}$ -matrices associated to all the finite irreducible and, respectively, reducible reflection groups with no more than four independent basic invariants. The results will be obtained using the explicit form of the basic invariant polynomials of the reflection groups that can be found in the mathematical and physical literature. A comparison of our results with the allowable solutions of the canonical equation reported in I and II will allow us to identify generating groups for all the irreducible, and some of the reducible, allowable  $\hat{P}$ -matrices.

After a few concluding remarks on our mathematical results, collected in §5, in the last section we shall illustrate how they can be used in one of the specific physical contexts mentioned in the introduction. Our aim will be to show that, despite the sophisticated mathematical tools that have been used to achieve the results presented in the paper, their practical exploitation in physical contexts only requires an elementary use of standard analysis, geometry and group theory. The physical problem we shall deal with in §6 has been studied by various authors in the past [53]; our revisitation will not lead to essentially new results, but for the fact that the explicit knowledge of the algebraic relations defining the strata will allow us to arrive at explicit analytic solutions in a particularly simple way.

## 2 An overview of the geometry of linear group actions

In this section, we shall first define most of our notations and recall, without proofs, some results concerning invariant theory and the geometry of orbit spaces of CLG's (see for instance [43, 44] and references therein), then we shall introduce the first definitions and the basic tools for our subsequent analysis.

For our purposes, it will not be restrictive to assume that  $G$  is a matrix subgroup of  $O_n(\mathbb{R})^3$  acting linearly in the Euclidean space  $\mathbb{R}^n$ .

### 2.1 Orbits and strata

We shall denote by  $x = (x_1, \dots, x_n)$  a point of  $\mathbb{R}^n$ . The group  $G$  acts in  $\mathbb{R}^n$  in the following way:

$$x'_i = (g \cdot x)_i = \sum_{j=1}^n g_{ij} x_j, \quad x \in \mathbb{R}^n, \quad g \in G. \quad (2)$$

The  $G$ -orbit  $\Omega_{\bar{x}}$  through  $\bar{x} \in \mathbb{R}^n$  and the *isotropy subgroup*  $G_{\bar{x}}$  of  $G$  at  $\bar{x} \in \mathbb{R}^n$  are defined by the following relations:

$$\Omega_{\bar{x}} = \{g \cdot \bar{x} \mid g \in G\}, \quad G_{\bar{x}} = \{g \in G \mid g \cdot \bar{x} = \bar{x}\}. \quad (3)$$

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<sup>3</sup>The stronger assumption  $G \subseteq SO_n(\mathbb{R})$  introduced in I and II is due to a slip; in fact, the unimodularity condition has never been used in these references.

The invariance of the Euclidean norm under orthogonal transformations assures that the  $G$ -orbit through  $\bar{x}$  is contained in the sphere of radius  $\bar{x}$ , centered in the origin of  $\mathbb{R}^n$ , while the linearity of the action of  $G$  in  $\mathbb{R}^n$  implies

$$G_{\bar{x}} = G_{\lambda\bar{x}}, \forall \lambda \in \mathbb{R}_*. \quad (4)$$

The isotropy subgroup of  $G$  at the origin of  $\mathbb{R}^n$  coincides with  $G$ . The isotropy subgroups  $G_{g\cdot\bar{x}}$  of  $G$ , at points lying on the same orbit  $\Omega_{\bar{x}}$  are conjugated subgroups in  $G$ :

$$G_{g\cdot\bar{x}} = gG_{\bar{x}}g^{-1}, \forall g \in G. \quad (5)$$

The class of all the subgroups of  $G$  conjugated to  $G_{\bar{x}}$  in  $G$  will be said to be the *orbit type* of  $\Omega_{\bar{x}}$  or, equivalently, of the points of  $\Omega_{\bar{x}}$ ; it specifies the symmetry properties of  $\Omega_{\bar{x}}$  under transformations induced by elements of  $G$ .

The set of all the points  $x \in \mathbb{R}^n$  (or, equivalently, of all the orbits of  $G$ ) with the same orbit type form an *isotropy type stratum of the action of  $G$  in  $\mathbb{R}^n$* , hereafter called simply a *stratum of  $\mathbb{R}^n$* . All the connected components of a stratum are smooth iso-dimensional sub-manifolds of  $\mathbb{R}^n$ .

## 2.2 The orbit space

The *orbit space* of the action of  $G$  in  $\mathbb{R}^n$  is defined as the quotient space  $\mathbb{R}^n/G$  (obtained through the equivalence relation between points belonging to the same orbit) endowed with the quotient topology and differentiable structure. We shall denote by  $\pi$  the canonical projection  $\mathbb{R}^n \rightarrow \mathbb{R}^n/G$ . Whole orbits of  $G$  are mapped by  $\pi$  into single points of  $\mathbb{R}^n/G$ . The image through  $\pi$  of a stratum of  $\mathbb{R}^n$  will be called an (*isotropy type*) *stratum of  $\mathbb{R}^n/G$* ; all its connected components turn out to be smooth iso-dimensional manifolds.

Almost all the points of  $\mathbb{R}^n/G$  belong to a unique stratum  $\Sigma_p$ , the *principal stratum*, which is a connected open dense subset of  $\mathbb{R}^n/G$ . The boundary  $\overline{\Sigma_p} \setminus \Sigma_p$  of  $\Sigma_p$  is the union of disjoint *singular* strata. All the strata lying on the boundary  $\overline{\Sigma} \setminus \Sigma$  of a stratum  $\Sigma$  of  $\mathbb{R}^n/G$  are open in  $\overline{\Sigma} \setminus \Sigma$ .

The following partial ordering can be introduced in the set of all the orbit types:  $[H] < [K]$  if  $H$  is a subgroup of a subgroup of  $G$  conjugated with  $K$ . The orbit type  $[H]$  of a stratum  $\Sigma$  is contained in the orbit types  $[H_b]$  of all the strata  $\Sigma_b$  lying in its boundary; therefore, more peripheral strata of  $\mathbb{R}^n/G$  are formed by orbits with higher symmetry under  $G$  transformations. The number of distinct orbit types of  $G$  is finite and there is a unique minimum orbit type, the *principal orbit type*, corresponding to the principal stratum; there is also a unique maximum orbit type  $[G]$ , corresponding to the image through  $\pi$  of all the points of  $\mathbb{R}^n$ , which are invariant under  $G$ .

A faithful image of  $\mathbb{R}^n/G$  can be obtained making use of a basic result of the geometric approach to invariant theory in the following way.

A function  $f(x)$  is said to be  $G$ -invariant if

$$f(g \cdot x) = f(x), \quad \forall x \in \mathbb{R}^n, g \in G. \quad (6)$$

The set of all real,  $G$ -invariant, polynomial functions of  $x$  forms a ring  $\mathbb{R}[x]^G$ , that admits a finite integrity basis [45, 46]. Therefore, there exists a finite minimal collection of invariant polynomials  $p(x) = (p_1(x), p_2(x), \dots, p_q(x))$  such that any element  $F \in \mathbb{R}[x]^G$  can be expressed as a polynomial function  $\hat{F}$  of  $p(x)$ :

$$\hat{F}(p(x)) = F(x), \forall x \in \mathbb{R}^n. \quad (7)$$

The polynomial  $\hat{F}(p)$  will be said to have weight  $w$ , if  $w$  is the degree of the polynomial  $F(x)$ ; it will be said to be  $w$ -homogeneous if such is  $F(x)$ .

The elements of a (minimal) basis of  $\mathbb{R}[x]^G$  can be chosen to be homogeneous polynomials. The number  $q$  of elements of a minimal integrity basis and their homogeneity *degrees*  $d_i$ 's are only determined by the group  $G$ .

To avoid trivial situations, in this paper we shall only consider linear groups with no fixed points, but for the origin of  $\mathbb{R}^n$ . In this case, the minimum degree of the elements of a minimal integrity basis is necessarily 2, and the following conventions can be adopted:

$$d_1 \geq d_2 \geq \dots d_q = 2; \quad p_q(x) = \|x\|^2 = \sum_1^n x_i^2. \quad (8)$$

Hereafter, by a minimal integrity basis of  $G$  (abbreviated into MIB of  $G$ ) we shall always mean a *minimal homogeneous integrity basis* for the ring of  $G$ -invariant polynomials, for which the conventions of (8) hold true.

Since  $G$  is a compact group, the orbits of  $G$  are separated by the elements of a MIB of  $G$ , i.e., at least one element of a MIB of  $G$  takes on different values on two distinct orbits. Thus, the elements of a MIB of  $G$  provide a good parametrization of the points of  $\mathbb{R}^n/G$ , that turns out to be also smooth, since the orbit map  $p : \mathbb{R}^n \longrightarrow \mathbb{R}^q$ , which maps all the points of  $\mathbb{R}^n$  lying on an orbit of  $G$  onto a single point of  $\mathbb{R}^q$ , induces a diffeomorphism of  $\mathbb{R}^n/G$  onto a semialgebraic  $q$ -dimensional connected closed subset of  $\mathbb{R}^q$ .

### 2.3 Coregular and non-coregular groups

The group  $G$  is said to be *coregular* if the elements of its MIB's are algebraically, and therefore functionally, independent. If  $G$  is non-coregular, the elements of any one of its MIB's satisfy a certain number of algebraic identities in  $\mathbb{R}^n$ :

$$\hat{F}_A(p(x)) = 0, \quad A = 1, \dots, K. \quad (9)$$

The associated equations

$$\hat{F}_A(p) = 0, \quad A = 1, \dots, K, \quad (10)$$

define an algebraic variety in  $\mathbb{R}^q$ , which will be called the *variety  $\mathcal{Z}$  of the relations* (among the elements of the MIB). The number  $K$  will be said the *coregularity order* of  $G$ . If  $G$  is coregular, there are no relations among the elements of its MIB's, the coregularity order of  $G$  is zero and we shall set  $\mathcal{Z} = \mathbb{R}^q$ .

From now on, in this paper, we shall deal mainly with coregular CLG's.

## 2.4 The $\hat{P}(p)$ matrix

A characterization of the image  $p(\mathbb{R}^n)$  of the orbit space of  $G$  as a semi-algebraic variety can be easily obtained through a matrix  $\hat{P}(p)$ , defined only in terms of the  $G$ -invariant Euclidean scalar products between the gradients of the elements of the MIB  $\{p(x)\}$ :

$$P_{ab}(x) = \sum_i^n \frac{\partial p_a(x)}{\partial x_i} \cdot \frac{\partial p_b(x)}{\partial x_i} = \hat{P}_{ab}(p(x)) \quad a, b = 1, \dots, q; \quad (11)$$

where in the last member, use has been made of Hilbert's theorem, in order to express  $P_{ab}(x)$  as a polynomial function of  $p_1(x), \dots, p_q(x)$ .

The following fundamental theorem clarifies the meaning and points out the role of the matrix  $\hat{P}(p)$ :

**Theorem 2.1** *Let  $G$  a compact coregular subgroup of  $O_n(\mathbb{R})$ ,  $p$  the map  $\mathbb{R}^n \rightarrow \mathbb{R}^q$  defined by the homogeneous MIB  $\{p_1(x), p_2(x), \dots, p_q(x)\}$  and  $\hat{P}(p)$  the matrix defined in (11). Then  $\overline{\mathcal{S}} = p(\mathbb{R}^n)$  is the unique semialgebraic connected subset of the variety  $\mathcal{Z} \subseteq \mathbb{R}^q$  of the relations among the elements of the MIB where  $\hat{P}(p)$  is positive semi-definite. The  $k$ -dimensional primary strata of  $\overline{\mathcal{S}}$  are the connected components of the set  $\widehat{W}^{(k)} = \{p \in \mathcal{Z}; | \hat{P}(p) \geq 0, \text{rank}(\hat{P}(p)) = k\}$ ; they are the images of the connected components of the  $k$ -dimensional isotropy type strata of  $\mathbb{R}^n/G$ . In particular the variety  $\mathcal{S}$  of the interior points of  $\overline{\mathcal{S}}$ , where  $\hat{P}(p)$  has the maximum rank, is the image of the principal stratum.*

It will be worthwhile to note that, for coregular groups,  $\mathcal{Z} = \mathbb{R}^q$  and that the image of the unit sphere of  $\mathbb{R}^n$  under the orbit map  $p(x)$  is a compact connected  $(q-1)$ -dimensional semialgebraic variety in the space  $\mathbb{R}^{q-1}$  spanned by the variables  $p_1, \dots, p_{q-1}$ .

The following properties, which are common to all the matrices  $\hat{P}(p)$ , are more or less immediate consequences of the definition of these matrices:

**P1** *Symmetry, homogeneity and bounds on the last row and column:* The matrix  $\hat{P}(p)$  is a  $q \times q$  symmetric matrix, whose elements  $\hat{P}_{ab}(p)$  are real w-homogeneous polynomials with weight

$$w(\hat{P}_{ab}) = d_a + d_b - 2. \quad (12)$$

The last row and column are determined by the degrees of the MIB:

$$\hat{P}_{qa}(p) = \hat{P}_{aq}(p) = 2d_a p_a, \quad a = 1, 2, \dots, q. \quad (13)$$

**P2** *Tensor character:* The matrix elements of  $\hat{P}(p)$  transform as the components of a rank 2 contravariant tensor under MIB transformations that maintain the conventions fixed in (8) (these transformations will be hereafter called MIBT's). In fact, let  $\{p(x)\}$  and  $\{p'(x)\}$  be distinct MIB's; the  $p'_a(x)$ 's, being  $G$ -invariant polynomials, can be expressed as polynomial functions of the  $p_a(x)$ 's:

$$p'_\alpha = p'_\alpha(p) \quad \alpha = 1, 2, \dots, q-1, \quad (14)$$

where the polynomial function  $p'_\alpha(p)$  only depends on the  $p_a$ 's such that<sup>4</sup>  $d_a \leq d'_\alpha$ . Then,

$$\hat{P}'(p'(p)) = J(p) \cdot \hat{P}(p) \cdot J^T(p), \quad (15)$$

where we have denoted by  $J(p)$  the Jacobian matrix of the transformation:

$$J_{ab}(p) = \partial p'_a(p) / \partial p_b, \quad a, b = 1, \dots, q; \quad (16)$$

the matrix  $J$  turns out to be upper-block triangular and the determinant of  $\hat{P}(p)$  to be a relative invariant of the group of the MIBT's.

## 2.5 Classification of the orbit spaces of CCLG's

Two matrices  $\hat{P}(p)$  and  $\hat{P}'(p')$  will be said to be *equivalent* if they are connected by a relation like (15), where  $J(p)$  is the Jacobian matrix of a MIBT  $p' = p'(p)$ . Thus, the  $\hat{P}$ -matrices computed from different MIB's of the same CLG are equivalent, and the semialgebraic varieties  $\overline{\mathcal{S}}$  and  $\overline{\mathcal{S}'}$  defined by the positivity conditions imposed on  $\hat{P}(p)$  and  $\hat{P}'(p')$  respectively, are equivalent concrete realizations of the orbit space  $\mathbb{R}^n/G$ .

Since  $G$  is coregular, its orbit space is completely determined by the positivity conditions of a  $\hat{P}$ -matrix computed from any one of its MIB's; for non-coregular groups, also a complete set of relations among the  $p_a$ 's has to be specified.

## 2.6 Isomorphism classes of orbit spaces

The notions of MIBT's (see (14)) and of equivalence of  $\hat{P}$ -matrices (see (15)) can be extended to the case of different coregular groups  $G$  and  $G'$ , provided that their MIB's have the same number of elements, with the same degrees. Let,  $\{p\}$  and  $\{p'\}$  be MIB's for  $G$  and  $G'$ , respectively.

**Definition 2.1** *The orbit space  $\mathbb{R}^n/G$  and  $\mathbb{R}^n/G'$  of the compact coregular linear groups  $G$  and  $G'$  will be said to be isomorphic if the associated  $\hat{P}$ -matrices  $\hat{P}(p)$  and  $\hat{P}'(p')$  satisfy (15), where the transformation  $p' = p'(p)$  has all the formal properties of a MIBT.*

If  $G$  and  $G'$  have isomorphic orbit spaces, then the images of their orbit spaces  $\overline{\mathcal{S}}$  and  $\overline{\mathcal{S}'}$ , associated with the MIB's  $\{p\}$  and  $\{p'\}$  are isomorphic semialgebraic varieties:

$$\overline{\mathcal{S}'} = p'(\overline{\mathcal{S}}). \quad (17)$$

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<sup>4</sup>Since in our conventions the  $q$ -th element of any MIB is fixed to equal  $\sum_{i=1}^n x_i^2$ , when defining a MIBT we shall always understand the condition  $p'_q(p) = p_q$ .

Thus the classification of the isomorphism classes of the orbit spaces of the CCLG's rests on the determination of a representative for each class of equivalent  $\hat{P}(p)$  matrices (and, for non-coregular groups, on the determination of the possible relations among the elements of the MIB's). This can be done, in principle, for all CCLG's. The matrices  $\hat{P}(p)$  have been shown [36], in fact, to be solutions of a *canonical differential equation*, satisfying convenient initial conditions (*allowable* solutions). The canonical equation does involve only the degrees  $\{d_1, d_2, \dots, d_q\}$  of the MIB's as free parameters, as we shall see in the next subsection.

## 2.7 Boundary and positivity conditions

The orbit space  $\overline{\mathcal{S}}$ , defined in Theorem (2.1), is a connected  $q$ -dimensional semialgebraic variety of  $\mathbb{R}^q$  and, like all semialgebraic varieties [47], it presents a natural stratification in connected semialgebraic sub-varieties  $\hat{\sigma}$ , called *primary strata*<sup>5</sup>. We shall denote by  $\mathcal{I}(\hat{\sigma})$  the ideal formed by all the polynomials in  $p \in \mathbb{R}^q$  vanishing on  $\hat{\sigma}$ . Every  $\hat{f}(p) \in \mathcal{I}(\hat{\sigma})$  defines an invariant polynomial function in  $\mathbb{R}^n$  vanishing at all the points  $x$  lying in the set  $\Sigma_f = p^{-1}(\hat{\sigma})$ :

$$f(x) = \hat{f}(p(x)) = 0, \quad \forall x \in \Sigma_f. \quad (18)$$

The gradient  $\partial f(x)$  is obviously orthogonal to  $\Sigma_f$  at every  $x \in \Sigma_f$ , but, it must also be tangent to  $\Sigma_f$  since  $f(x)$  is a G-invariant function [43, 24]. As a consequence,

$$0 = \partial f(x) = \sum_1^q \partial_b \hat{f}(p) \Big|_{p=p(x)} \cdot \partial p_b(x), \quad \forall x \in \Sigma_f. \quad (19)$$

By taking the scalar product of (19) with  $\partial p_a(x)$ , we end up with the following *boundary conditions* [38]:

$$\sum_1^q \partial_b \hat{P}_{ab}(p) \partial_b \hat{f}(p) \in \mathcal{I}(\hat{\sigma}), \quad \forall \hat{f} \in \mathcal{I}(\hat{\sigma}) \text{ and } \forall \hat{\sigma} \subseteq \overline{\mathcal{S}}. \quad (20)$$

If  $\{Q_1^{(\hat{\sigma})}(p), Q_2^{(\hat{\sigma})}(p), \dots, Q_m^{(\hat{\sigma})}(p)\}$  is an integrity basis for  $\mathcal{I}(\hat{\sigma})$ , (20) is equivalent to:

$$\sum_1^q \partial_b \hat{P}_{ab}(p) \partial_b Q_r^{(\hat{\sigma})}(p) = \sum_1^m \lambda_{rs;a}^{(\hat{\sigma})}(p) Q_s^{(\hat{\sigma})}(p), \quad (21)$$

where the  $\lambda$ 's are  $w$ -homogeneous polynomial functions of  $p$ .

In the particular case in which  $\hat{\sigma}$  is a  $(q-1)$ -dimensional primary stratum, the ideal  $\mathcal{I}(\hat{\sigma})$  has a unique *irreducible* generator,  $Q^{(\hat{\sigma})}(p)$ , and (21) reduces to the simpler form [36, 38]

$$\sum_1^q \partial_b \hat{P}_{ab}(p) \partial_b Q^{(\hat{\sigma})}(p) = \lambda_a^{(\hat{\sigma})}(p) Q^{(\hat{\sigma})}(p), \quad a = 1, \dots, q. \quad (22)$$

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<sup>5</sup> A simple example of a compact connected semialgebraic variety of  $\mathbb{R}^3$  is yielded by a polyhedron. Its interior points form its unique 3-dimensional primary stratum, while 2-, 1- and 0-dimensional primary strata are formed, respectively, by the interior points of each face, by the interior points of each edge, by each vertex.

The validity of (21) can be extended to the case in which  $\hat{\sigma}$  is a union of primary strata. In particular, the ideal  $\mathcal{I}(\mathcal{B})$ , associated to the union  $\mathcal{B}$  of all the  $(q-1)$ -dimensional strata of  $\overline{\mathcal{S}}$  (whose closure forms the boundary of  $\overline{\mathcal{S}}$ ) has a unique generator  $A(p)$ :

$$A(p) = \prod_{\hat{\sigma} \subseteq \mathcal{B}} Q^{(\hat{\sigma})}(p) \quad (23)$$

and the following relation is satisfied:

$$\sum_1^q {}_b\hat{P}_{ab}(p) \partial_b A(p) = \lambda_a^{(A)}(p) A(p), \quad (24)$$

where  $\lambda^{(A)}(p)$  is a contravariant vector field with  $w$ -homogeneous components, and

$$\lambda^{(A)}(p) = \sum_{\hat{\sigma} \subseteq \mathcal{B}} \lambda^{(\hat{\sigma})}(p). \quad (25)$$

The results summarized below have been proved in [37].

The vector  $\lambda^{(A)}(p)$  can be reduced to the canonical form  $\lambda_a^{(A)}(p) = 2\delta_{aq}w(A)$  in particular MIB's, the so-called *A-bases*, which are intrinsically defined. In an *A*-basis, the boundary conditions assume the following *canonical* form:

$$\sum_1^q {}_b\hat{P}_{ab}(p) \partial_b A(p) = 2\delta_{aq}w(A)A(p), \quad a = 1, \dots, q. \quad (26)$$

From (26) one deduces that, in every *A*-basis, the following facts hold true:

- i) The point  $p^{(0)} = (0, \dots, 0, 1)$  lies in  $\mathcal{S}$ ; it is the image of a  $G$ -orbit lying on the unit sphere of  $\mathbb{R}^n$ .
- ii)  $A(p)$  is a factor of  $\det \hat{P}(p)$ ; its weight is bounded:

$$2d_1 \leq w(A) \leq w(\det \hat{P}) = 2 \sum_1^q d_a - 2q \quad (27)$$

and it can be normalized at  $p^{(0)}$ :

$$A(p^{(0)}) = 1; \quad (28)$$

we shall call it the *complete active factor* of  $\det \hat{P}(p)$ .

- iii) The restriction,  $A(p)|_{p_q=1}$ , of  $A(p)$  to the image of the unit sphere of  $\mathbb{R}^n$  in  $\mathbb{R}^q$  has a unique local non degenerate maximum lying at  $p^{(0)}$ ; thus:

$$\partial_\alpha A(p)|_{p=p^{(0)}} = 0, \quad \alpha = 1, \dots, q-1. \quad (29)$$

iv)  $\hat{P}(p^{(0)})$  is block diagonal, each block being associated to a subset of  $p_a$ 's sharing the same degree, and, in a subclass of  $A$ -bases (*standard A-bases*), it is diagonal:

$$\hat{P}_{ab}(p^{(0)}) = d_a d_b \delta_{ab}, \quad a, b = 1, \dots, q. \quad (30)$$

Two different standard  $A$ -bases are related by a MIBT not involving  $p_q$ :

$$p'_\alpha = f_\alpha(p_1, \dots, p_{q-1}), \quad \alpha = 1, \dots, q-1; \quad (31)$$

the corresponding Jacobian matrix is orthogonal at  $p^{(0)}$ .

## 2.8 The canonical equation

Let us now look at the boundary conditions from a different point of view: the set  $\{p_1, \dots, p_q\}$  will be viewed as a set of *weighted indeterminates*, with integer weights  $d_1, \dots, d_q$  satisfying the conventions

$$d_1 \geq d_2 \geq \dots d_q = 2; \quad (32)$$

and the boundary conditions expressed in (26) will be considered as a set of equations in which  $\hat{P}_{ab}(p)$  and  $A(p)$  are thought of as unknown polynomial functions of  $p$ , satisfying the conditions listed under items **P1-P2** and in (27). The positivity conditions specified in (28) and (30) will be treated as initial conditions. With the above meaning for the symbols, (26) will be called the *canonical equation*.

The solutions  $(\hat{P}(p), A(p))$  of the canonical equation satisfying the initial conditions specified in (28) and (30) will be called *allowable solutions* and the corresponding  $\hat{P}$  matrices, *allowable  $\hat{P}$  matrices*.

A solution of the canonical equation will be said to be *irreducible*, if  $A(p)$  is an irreducible (real) polynomial and *fully active*, if  $A(p) = \text{const} \cdot \det \hat{P}(p)$ .

Two allowable  $\hat{P}$  matrices will be said to be equivalent if a  $w$ -homogeneous transformation exists on the indeterminates  $p_1, \dots, p_{q-1}$  such that (15) is satisfied.

The allowable  $\hat{P}$ -matrices  $\hat{P}(p)|_{p_q=1}$  have been shown to be positive semi-definite only in a compact  $(q-1)$ -dimensional semialgebraic variety of the space  $\mathbb{R}^{q-1}$  spanned by the variables  $p_1, \dots, p_{q-1}$ , containing the point  $p^{(0)}$ .

All the  $\hat{P}$ -matrices associated to the different MIB's of any CCLG with no fixed points are necessarily equivalent to an allowable  $\hat{P}$ -matrix. At present we do not know if the converse holds also true, i.e., if every allowable  $\hat{P}$ -matrix is generated by a CCLG with no fixed points.

The allowable solutions of the canonical equations for  $q \leq 4$  have been determined in I and II. For each choice of the degrees  $\{d_1, d_2, \dots, d_q\}$ , only a finite or null number of non equivalent solutions has been found, showing the existence of *selection rules* for the degrees of the CCLG's. The solutions can be organized in *towers*; the degrees of the elements of the same tower can be written in the form  $d_\alpha = s d_\alpha^{(0)}$ ,  $\alpha = 1, \dots, q-1$ , where  $s$  is an integer

scale parameter. A solution of the canonical equation corresponding to  $s = 1$  will be said a *fundamental* solution.

Exploiting the fact that all the *finite* coregular linear groups have been classified in the mathematical literature and the associated MIB's have been determined [48], in the following sections we shall determine the  $\hat{P}$ -matrices of all the finite CLG's with 2-, 3- [38] and 4-dimensional [39] orbit spaces, and we shall check that they can all be found among the allowable solutions of the canonical equation listed in I and II.

### 3 Irreducible reflection groups with 2, 3 and 4 basic invariants

Finite groups generated by reflections exhaust the class of *finite* CLG's. The explicit form of the elements of at least one MIB is known for all these groups [27, 28, 29, 30, 31, 32]. Thus, the corresponding  $\hat{P}(p)$  matrices can be computed, as well as the complete factors  $A(p)$  of  $\det \hat{P}(p)$  and the vector fields  $\lambda^{(A)}(p)$  appearing in (24).

In general, the MIB's proposed in the literature do not correspond to  $A$ -bases, so the comparison with the results reported in I and II is not immediate. The easiest way to determine the form of a MIBT leading to an  $A$ -basis is through the following condition on the Jacobian matrix  $J_{ab}(p)$  of the transformation:

$$\lambda_a^{(A)}(p'(p)) = \sum_b^q J_{ab}(p) \lambda_b^{(A)}(p) = 0, \quad a = 1, 2, \dots, (q-1). \quad (33)$$

When the  $A$ -basis is not unique, (33) is not sufficient to determine all the free parameters involved in the definition of the MIBT. The residual free parameters can however be determined by requiring that the parametric expression of  $\hat{P}'(p')$  in a general  $A$ -basis coincides with an allowable  $\hat{P}$ -matrix listed in I or II. To shorten our formulas and to make easier the comparison, we shall define

$$\tilde{p} = (p_1, \dots, p_{q-1}, 1), \quad \text{for } p = (p_1, \dots, p_q), \quad (34)$$

$$\tilde{x} = (x_1, \dots, x_n, 0), \quad \text{for } x = (x_1, \dots, x_n), \quad (35)$$

$$R_{ab} = \hat{P}_{ab}/d_a d_b, \quad a, b = 1, \dots, q, \quad (36)$$

$$f_{n,k}(x) = \sum_i^n x_i^{n+1-k}, \quad \text{for } x = (x_1, \dots, x_n). \quad (37)$$

#### 3.1 Irreducible CCLG's with 2 basic invariants

The irreducible CCLG's with 2-dimensional orbit spaces are classified in the mathematical literature according to the following *types*:  $A_2$ ,  $B_2$ ,  $G_2$  and  $I_2(m)$ . The type  $G_2$  and  $I_2(6)$  groups have the same invariants, so we shall not discuss separately the group of type  $G_2$ .

### 3.2 Type A<sub>2</sub>

The group acts on the plane  $y_1 + y_2 + y_3 = 0$  of  $\mathbb{R}^3$  by permutations. Therefore the group and its invariants can be obtained from the reduction of the group  $S_3$ , acting on  $y = (y_1, y_2, y_3)$  by permutations of the coordinates.

A MIB for  $S_3$  is yielded by  $\{f_{3,1}(y), f_{3,2}(y), f_{3,3}(y)\}$ , where  $f_{3,k}$  is defined in (37). The reduction of the linear group  $S_3$  can be obtained by means of an orthogonal basis transformation in  $\mathbb{R}^3$ , induced by the matrix

$$A = \frac{1}{6} \begin{pmatrix} \sqrt{3} & -\sqrt{3} & 0 \\ 1 & 1 & -2 \\ \sqrt{2} & \sqrt{2} & \sqrt{2} \end{pmatrix}. \quad (38)$$

The elements of the linear group of type A<sub>2</sub> are obtained as the principal minors built with the first 2 rows and columns of the matrices  $AgA^{-1}$ ,  $g \in S_3$  and, after setting, for  $x = (x_1, \dots, x_n)$ ,

$$p_a(x) = \tilde{p}_a(A^{-1}\tilde{x}), \quad (39)$$

and  $x = (x_1, x_2)$ , a MIB for A<sub>2</sub> is yielded by  $\{p_1(x), p_2(x)\}$  or, explicitly:

$$\begin{aligned} p_1(x) &= x_2 (3x_1^2 - x_2^2) / \sqrt{6}, \\ p_2(x) &= x_1^2 + x_2^2. \end{aligned} \quad (40)$$

The unique element of the associated reduced  $\hat{P}$ -matrix is easily calculated to be

$$\hat{P}_{11}(p) = 3p_2^2/2 \quad (41)$$

and after the following MIBT:

$$p'_1 = \sqrt{6} p_1, \quad (42)$$

one obtains, for  $p'_2 = 1$ , the allowable  $\hat{P}(p)$  matrix determined in I for  $q = 2$  and  $d_1 = 3$ :

$$R'_{11}(\tilde{p}') = 1. \quad (43)$$

### 3.3 Type B<sub>2</sub>

The group acts on  $x = (x_1, x_2)$  by permutations and sign changes of the coordinates. A MIB can be chosen as follows:

$$\begin{aligned} p_1(x) &= x_1^4 + x_2^4, \\ p_2(x) &= x_1^2 + x_2^2. \end{aligned} \quad (44)$$

The unique essential element of the associated  $\hat{P}$ -matrix turns out to be the following

$$\hat{P}_{11}(p) = 8p_2(3p_1 - p_2^2) \quad (45)$$

and after the following MIBT:

$$p'_1 = 4p_1 - 3p_2^2, \quad (46)$$

one obtains, for  $p'_2 = 1$ , the allowable  $\hat{R}(p)$  matrix determined in I for  $q = 2$  and  $d_1 = 4$ :

$$R'_{11}(\tilde{p}') = 1. \quad (47)$$

### 3.4 Type $I_2(m)$ , $m \geq 3$

The groups of type  $I_2(m)$ ,  $m \geq 3$ , are the dihedral groups  $\mathcal{D}_m$ , defined as the groups of orthogonal transformations of  $\mathbb{R}^2$  which preserve a regular  $m$ -sided polygon centered at the origin. After setting

$$z = x_1 + ix_2, \quad (48)$$

a MIB of  $\mathcal{D}_m$  is yielded, for instance, by the invariants  $p(x) = \{p_1(x), p_2(x)\}$ , with

$$p_1(x) = \Re z^m, \quad p_2(x) = |z|^2 = x_1^2 + x_2^2. \quad (49)$$

The unique essential element of the associated  $\hat{P}$ -matrix turns out to be the following:

$$\hat{P}_{11}(p) = d_1^2 p_2^{m-1}. \quad (50)$$

A comparison with I shows that  $\{p\}$  is a standard A-basis.

### 3.5 Type $A_3$

The group acts on the plane  $y_1 + y_2 + y_3 + y_4 = 0$  of  $\mathbb{R}^4$  by permutations. Therefore the group and its invariants can be obtained from the reduction of the group  $S_4$ , acting on  $y = (y_1, y_2, y_3, y_4)$  by permutations of the coordinates.

A MIB for  $S_4$  is yielded by  $\{f_1(y), \dots, f_4(y)\}$ , where  $f_k$  is defined in (37). The reduction of the linear group  $S_4$  can be obtained by means of an orthogonal basis transformation in  $\mathbb{R}^4$ , induced by the matrix

$$A = \frac{1}{6} \begin{pmatrix} 3\sqrt{2} & -3\sqrt{2} & 0 & 0 \\ \sqrt{6} & \sqrt{6} & -2\sqrt{6} & 0 \\ \sqrt{3} & \sqrt{3} & \sqrt{3} & -3\sqrt{3} \\ 3 & 3 & 3 & 3 \end{pmatrix}. \quad (51)$$

The elements of the group of type  $A_3$  are obtained as the principal minors built with the first 3 rows and columns of the matrices  $AgA^{-1}$ ,  $g \in S_4$  and, after setting  $x = (x_1, x_2, x_3)$ , a MIB is yielded by  $\{p_1(x), p_2(x), p_3(x)\}$ , with  $p_a(x)$  defined in (39); explicitly:

$$\begin{aligned} p_1(x) &= \left(6x_1^4 + 12x_1^2x_2^2 + 6x_2^4 + 12\sqrt{2}x_1^2x_2x_3 - 4\sqrt{2}x_2^3x_3 + 6x_1^2x_3^2 + 6x_2^2x_3^2 + 7x_3^4\right)/12, \\ p_2(x) &= \left(3\sqrt{2}x_1^2x_2 - \sqrt{2}x_2^3 + 3x_1^2x_3 + 3x_2^2x_3 - 2x_3^3\right)/2\sqrt{3}, \\ p_3(x) &= x_1^2 + x_2^2 + x_3^2. \end{aligned} \quad (52)$$

The essential elements of the associated  $\hat{P}(p)$ -matrix turn out to be the following:

$$\begin{aligned} \hat{P}_{11}(p) &= 2 \left(18p_1p_3 + 2p_2^2 - 3p_3^3\right)/3, \\ \hat{P}_{12}(p) &= 7p_2p_3, \\ \hat{P}_{22}(p) &= 9 \left(4p_1 - p_3^2\right)/4 \end{aligned} \quad (53)$$

and after the following MIBT:

$$\begin{aligned} p'_1 &= 12p_1 - 5p_3^2, \\ p'_2 &= 2\sqrt{3}p_2, \end{aligned} \quad (54)$$

one obtains, for  $p'_3 = 1$ , the matrix  $R$  of class III.1( $m = 1$ ), reported in I:

$$\begin{aligned} R'_{11}(\tilde{p}') &= -p'_1 + p'^2_2 + 2, \\ R'_{12}(\tilde{p}') &= 2p'_2, \\ R'_{22}(\tilde{p}') &= p'_1 + 2. \end{aligned} \quad (55)$$

### 3.6 Type $B_3$

The group acts on  $x = (x_1, x_2, x_3)$  by permutations and sign changes of the coordinates. A MIB can be chosen as follows:

$$\begin{aligned} p_1(x) &= x_1^6 + x_2^6 + x_3^6, \\ p_2(x) &= x_1^4 + x_2^4 + x_3^4, \\ p_3(x) &= x_1^2 + x_2^2 + x_3^2. \end{aligned} \quad (56)$$

The essential elements of the associated  $\hat{P}(p)$ -matrix turn out to be the following:

$$\begin{aligned}
\hat{P}_{11}(p) &= 30p_1p_2 + 30p_1p_3^2 - 30p_2p_3^3 + 6p_3^5, \\
\hat{P}_{12}(p) &= 32p_1p_3 + 12p_2^2 - 24p_2p_3^2 + 4p_3^4, \\
\hat{P}_{22}(p) &= 16p_1.
\end{aligned} \tag{57}$$

and after the following MIBT:

$$\begin{aligned}
p'_1 &= 324p_1 - 432p_2p_3 + 124p_3^3, \\
p'_2 &= 18p_2 - 10p_3^2,
\end{aligned} \tag{58}$$

one obtains, for  $p'_3 = 1$ , the matrix  $R$  of class III.2( $m = 1$ ) reported in I:

$$\begin{aligned}
R'_{11}(\tilde{p}') &= -p'_1p'_2 - 4p'_1 + 8p'^2_2 - 16p'_2 + 64, \\
R'_{12}(\tilde{p}') &= -2p'_1 + p'^2_2 + 12p'_2, \\
R'_{22}(\tilde{p}') &= p'_1 + 4p'_2 + 16.
\end{aligned} \tag{59}$$

### 3.7 Type $D_3$

The group acts on  $x = (x_1, x_2, x_3)$  by permutations and by changes of an even number of signs of the coordinates. A MIB can be chosen as follows:

$$\begin{aligned}
p_1 &= x_1^4 + x_2^4 + x_3^4, \\
p_2 &= x_1 x_2 x_3, \\
p_3 &= x_1^2 + x_2^2 + x_3^2.
\end{aligned} \tag{60}$$

The essential elements of the associated  $\hat{P}$ -matrix turn out to be the following:

$$\begin{aligned}
\hat{P}_{11}(p) &= 24p_1p_3 + 48p_2^2 - 8p_3^3, \\
\hat{P}_{12}(p) &= 4p_2p_3, \\
\hat{P}_{22}(p) &= (-p_1 + p_3^2)/2
\end{aligned} \tag{61}$$

and, after the following MIB transformation:

$$\begin{aligned}
p'_1 &= 4p_3^2 - 6p_1, \\
p'_2 &= 6\sqrt{3}p_2,
\end{aligned} \tag{62}$$

one obtains, for  $p'_3 = 1$ , the matrix  $R$  of class III.1( $m = 1$ ) reported in I. The orbit spaces of the linear groups  $A_3$  and  $D_3$  turn out to be isomorphic.

### 3.8 Type $H_3$

The group is the symmetry group of the icosahedron in  $\mathbb{R}^3$ .

Let us denote by  $\tau$  the golden ratio:

$$\tau = (1 + \sqrt{5})/2. \quad (63)$$

Then, according to [31], a MIB for the group can be chosen as follows:

$$\begin{aligned} p_1(x) &= (1 + \tau^2)^{-5} \left[ (1 + \tau^{10})(x_1^{10} + x_2^{10} + x_3^{10}) + 45\tau^2(x_1^2x_2^8 + x_2^2x_3^8 + x_3^2x_1^8) \right. \\ &\quad \left. + 210\tau^4(x_1^4x_2^6 + x_2^4x_3^6 + x_3^4x_1^6) + 210\tau^6(x_1^6x_2^4 + x_2^6x_3^4 + x_3^6x_1^4) \right. \\ &\quad \left. + 45\tau^8(x_1^8x_2^2 + x_2^8x_3^2 + x_3^8x_1^2) \right], \\ p_2(x) &= (1 + \tau^2)^{-3} \left[ (1 + \tau^6)(x_1^6 + x_2^6 + x_3^6) + 15\tau^2(x_1^2x_2^4 + x_2^2x_3^4 + x_3^2x_1^4) \right. \\ &\quad \left. + 15\tau^4(x_1^4x_2^2 + x_2^4x_3^2 + x_3^4x_1^2) \right], \\ p_3(x) &= x_1^2 + x_2^2 + x_3^2. \end{aligned} \quad (64)$$

The essential elements of the associated  $\hat{P}$ -matrix turn out to be the following:

$$\begin{aligned} \hat{P}_{11}(p) &= 192p_1p_2p_3 + 336p_1p_3^4/5 + 16p_2^3/9 - 1136p_2^2p_3^3/15 - 15968p_2p_3^6/75 \\ &\quad + 81412p_3^9/1125, \\ \hat{P}_{12}(p) &= 336p_1p_3^2/5 + 184p_2^2p_3/3 - 404p_2p_3^4/3 + 2656p_3^7/75, \\ \hat{P}_{22}(p) &= 18p_1 - 12p_2p_3^2 + 174p_3^5/25, \end{aligned} \quad (65)$$

and, after the following MIBT:

$$\begin{aligned} p'_1 &= (50625p_1 - 123750p_2p_3^2 + 39285p_3^5)/2, \\ p'_2 &= 225p_2 - 93p_3^3, \end{aligned} \quad (66)$$

one obtains, for  $p'_3 = 1$ , the matrix  $R$  of class III.3( $m = 1$ ) reported in I:

$$\begin{aligned} R'_{11}(\tilde{p}') &= 1152 - 12p'_1 - 168p'_2 - 4p'_1p'_2 + 44p'^2_2 + p'^3_2, \\ R'_{12}(\tilde{p}') &= -6p'_1 + 60p'_2 + 5p'^2_2, \\ R'_{22}(\tilde{p}') &= 96 + p'_1 + 14p'_2, \end{aligned} \quad (67)$$

### 3.9 Type $A_4$

The group acts on the plane  $y_1 + y_2 + y_3 + y_4 + y_5 = 0$  of  $\mathbb{R}^5$  by permutations. Therefore the group and its invariants can be obtained from the reduction of the group  $S_5$ , acting on  $y = (y_1, \dots, y_5)$  by permutations of the coordinates.

A MIB for  $S_5$  is yielded by  $\{f_{5,1}(y), \dots, f_{5,5}(y)\}$ , where  $f_{5,k}$  is defined in (37). The reduction of the linear group  $S_5$  can be obtained by means of an orthogonal basis transformation in  $\mathbb{R}^5$ , induced by the matrix

$$A = \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 & 0 & 0 \\ \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & -\frac{2}{\sqrt{6}} & 0 & 0 \\ \frac{1}{2\sqrt{3}} & \frac{1}{2\sqrt{3}} & \frac{1}{2\sqrt{3}} & -\frac{3}{2\sqrt{3}} & 0 \\ \frac{1}{2\sqrt{5}} & \frac{1}{2\sqrt{5}} & \frac{1}{2\sqrt{5}} & \frac{1}{2\sqrt{5}} & -\frac{4}{2\sqrt{5}} \\ \frac{1}{\sqrt{5}} & \frac{1}{\sqrt{5}} & \frac{1}{\sqrt{5}} & \frac{1}{\sqrt{5}} & \frac{1}{\sqrt{5}} \end{pmatrix}. \quad (68)$$

The elements of the group of type  $A_4$  are obtained as the principal minors built with the first 4 rows and columns of the matrices  $AgA^{-1}$ ,  $g \in S_5$  and, after setting  $x = (x_1, \dots, x_4)$ , a MIB is yielded by  $\{p_1(x), \dots, p_4(x)\}$ , where  $p_a(x)$  is defined in (39); explicitly:

$$\begin{aligned} p_1(x) &= 1800^{-1} \left( 750\sqrt{6}x_1^4x_2 + 500\sqrt{6}x_1^2x_2^3 - 250\sqrt{6}x_2^5 + 750\sqrt{3}x_1^4x_3 + 1500\sqrt{3}x_1^2x_2^2x_3 \right. \\ &\quad + 750\sqrt{3}x_2^4x_3 + 750\sqrt{6}x_1^2x_2x_3^2 - 250\sqrt{6}x_2^3x_3^2 + 250\sqrt{3}x_1^2x_3^3 + 250\sqrt{3}x_2^2x_3^3 \\ &\quad - 500\sqrt{3}x_3^5 + 450\sqrt{5}x_1^4x_4 + 900\sqrt{5}x_1^2x_2^2x_4 + 450\sqrt{5}x_2^4x_4 + 900\sqrt{10}x_1^2x_2x_3x_4 \\ &\quad - 300\sqrt{10}x_2^3x_3x_4 + 450\sqrt{5}x_1^2x_3^2x_4 + 450\sqrt{5}x_2^2x_3^2x_4 + 525\sqrt{5}x_3^4x_4 \\ &\quad + 450\sqrt{6}x_1^2x_2x_4^2 - 150\sqrt{6}x_2^3x_4^2 + 450\sqrt{3}x_1^2x_3x_4^2 + 450\sqrt{3}x_2^2x_3x_4^2 \\ &\quad \left. - 300\sqrt{3}x_3^3x_4^2 + 90\sqrt{5}x_1^2x_4^3 + 90\sqrt{5}x_2^2x_4^3 + 90\sqrt{5}x_3^2x_4^3 - 459\sqrt{5}x_4^5 \right), \\ p_2(x) &= 60^{-1} \left( 30x_1^4 + 60x_1^2x_2^2 + 30x_2^4 + 60\sqrt{2}x_1^2x_2x_3 - 20\sqrt{2}x_2^3x_3 + 30x_1^2x_3^2 + 30x_2^2x_3^2 \right. \\ &\quad + 35x_3^4 + 12\sqrt{30}x_1^2x_2x_4 - 4\sqrt{30}x_2^3x_4 + 121\sqrt{5}x_1^2x_3x_4 + 121\sqrt{5}x_2^2x_3x_4 \\ &\quad \left. - 81\sqrt{5}x_3^3x_4 + 18x_1^2x_4^2 + 18x_2^2x_4^2 + 18x_3^2x_4^2 + 39x_4^4 \right), \\ p_3(x) &= 30^{-1} \left( 15\sqrt{6}x_1^2x_2 - 5\sqrt{6}x_2^3 + 15\sqrt{3}x_1^2x_3 + 15\sqrt{3}x_2^2x_3 - 10\sqrt{3}x_3^3 + 9\sqrt{5}x_1^2x_4 \right. \\ &\quad \left. + 9\sqrt{5}x_2^2x_4 + 9\sqrt{5}x_3^2x_4 - 9\sqrt{5}x_4^3 \right), \\ p_4(x) &= x_1^2 + x_2^2 + x_3^2 + x_4^2. \end{aligned} \quad (69)$$

The essential elements of the associated  $\hat{P}(p)$ -matrix turn out to be the following:

$$\begin{aligned} \hat{P}_{11}(p) &= 5 \left( 12p_2^2 + 128p_1p_3 + 20p_2p_4^2 - 5p_4^4 \right) / 48, \\ \hat{P}_{12}(p) &= \left( 46p_2p_3 + 84p_1p_4 - 35p_3p_4^2 \right) / 6, \\ \hat{P}_{13}(p) &= \left( 40p_3^2 + 66p_2p_4 - 15p_4^3 \right) / 8, \\ \hat{P}_{22}(p) &= 2 \left( 16p_3^2 + 90p_2p_4 - 15p_4^3 \right) / 15, \end{aligned}$$

$$\begin{aligned}
\hat{P}_{23}(p) &= 12(5p_1 - p_3p_4)/5, \\
\hat{P}_{33}(p) &= 9(5p_2 - p_4^2)/5,
\end{aligned} \tag{70}$$

and, after the following MIBT:

$$\begin{aligned}
p'_1 &= 30\sqrt{15}(4p_1 - 3p_3p_4), \\
p'_2 &= 3(20p_2 - 7p_4^2), \\
p'_3 &= 6\sqrt{15}p_3,
\end{aligned} \tag{71}$$

one obtains, for  $p'_3 = 1$ , the matrix  $R$  of class  $E_1(s=1)$ , reported in II:

$$\begin{aligned}
R'_{11}(\tilde{p}') &= -4p'_1p'_3 + 3p'^2_2 - 27p'_2 + 18(2p'^2_3 + 9), \\
R'_{12}(\tilde{p}') &= -6p'_1 + p'_3(5p'_2 + 54), \\
R'_{13}(\tilde{p}') &= 2(3p'_2 + p'^2_3), \\
R'_{22}(\tilde{p}') &= 3p'_2 + 2(4p'^2_3 + 27), \\
R'_{23}(\tilde{p}') &= p'_1 + 12p'_3, \\
R'_{33}(\tilde{p}') &= p'_2 + 9.
\end{aligned} \tag{72}$$

### 3.10 Type $B_4$

The group acts on  $x = (x_1, x_2, x_3, x_4)$  by permutations and sign changes of the coordinates. A MIB can be chosen as follows:

$$\{p_a(x) = \sum_{i=1}^4 x_i^{10-2a}\}_{1 \leq a \leq 4}. \tag{73}$$

In this basis the essential elements of the  $\hat{P}(p)$  matrix turn out to be the following:

$$\begin{aligned}
\hat{P}_{11}(p) &= 4(28p_1p_2 + 14p_2p_3^2 + 42p_1p_3p_4 - 21p_3^3p_4 - 28p_2p_3p_4^2 + 14p_1p_4^3 + 7p_3^2p_4^3 - 14p_2p_4^4 \\
&\quad + 7p_3p_4^5 - p_4^7)/3, \\
\hat{P}_{12}(p) &= 16p_2^2 + 36p_1p_3 - 6p_3^3 + 36p_1p_4^2 - 18p_3^2p_4^2 - 32p_2p_4^3 + 18p_3p_4^4 - 2p_4^6, \\
\hat{P}_{13}(p) &= 4(20p_2p_3 + 30p_1p_4 - 15p_3^2p_4 - 20p_2p_4^2 + 10p_3p_4^3 - p_4^5)/3, \\
\hat{P}_{22}(p) &= 3(20p_2p_3 + 30p_1p_4 - 15p_3^2p_4 - 20p_2p_4^2 + 10p_3p_4^3 - p_4^5)/2, \\
\hat{P}_{23}(p) &= 24p_1, \\
\hat{P}_{33}(p) &= 16p_2,
\end{aligned} \tag{74}$$

and after the following MIBT:

$$\begin{aligned}
p'_1 &= 110592 p_1 - 55296 p_3^2 - 138240 p_2 p_4 + 98496 p_3 p_4^2 - 15066 p_4^4, \\
p'_2 &= 2304 p_2 - 2592 p_3 p_4 + 612 p_4^3, \\
p'_3 &= 48 p_3 - 21 p_4^2,
\end{aligned} \tag{75}$$

one obtains, for  $p'_4 = 1$ , the matrix  $R$  of class  $E3(s=1)$ , reported in II:

$$\begin{aligned}
R'_{11}(\tilde{p}') &= 2 p'_1 (p'_2 - 54) + 15 p'^2_2 + 216 p'_2 p'_3 + 324 (4 p'^2_3 + 18 p'_3 + 81), \\
R'_{12}(\tilde{p}') &= 6 p'_1 p'_3 - p'^2_2 + 18 p'_2 (p'_3 + 12) + 1620 p'_3, \\
R'_{13}(\tilde{p}') &= 6 p'_1 - p'_2 (p'_3 - 27) + 54 p'_3, \\
R'_{22}(\tilde{p}') &= 4 \left[ 3 p'_1 - p'_2 (p'_3 + 9) + 27 (p'^2_3 - 2 p'_3 + 27) \right], \\
R'_{23}(\tilde{p}') &= p'_1 - 3 p'_2 - 6 p'^2_3 + 108 p'_3, \\
R'_{33}(\tilde{p}') &= p'_2 - 12 p'_3 + 81.
\end{aligned} \tag{76}$$

### 3.11 Type $D_4$

The group acts on  $x = (x_1, x_2, x_3, x_4)$  by permutations and by changes of an even number of signs of the coordinates. A MIB can be chosen as follows:

$$p_1(x) = \sum_1^4 x_i^6, \quad p_2(x) = \sum_1^4 x_i^4, \quad p_3(x) = \prod_{i=1}^4 x_i, \quad p_4(x) = \sum_1^4 x_i^2. \tag{77}$$

The essential elements of the associated  $\hat{P}$ -matrix turn out to be the following:

$$\begin{aligned}
\hat{P}_{11}(p) &= 6(5p_1 p_2 - 30p_3^2 p_4 + 5p_1 p_4^2 - 5p_2 p_4^3 + p_4^5), \\
\hat{P}_{12}(p) &= 4(3p_2^2 - 24p_3^2 + 8p_1 p_4 - 6p_2 p_4^2 + p_4^4), \\
\hat{P}_{13}(p) &= 6p_2 p_3, \\
\hat{P}_{22}(p) &= 16p_1, \\
\hat{P}_{23}(p) &= 4p_3 p_4, \\
\hat{P}_{33}(p) &= (2p_1 - 3p_2 p_4 + p_4^3) / 6,
\end{aligned} \tag{78}$$

and, after the following MIBT:

$$\begin{aligned}
p'_1 &= 12 \left( 12 p_1 - 15 p_2 p_4 + 4 p_4^3 \right), \\
p'_2 &= 48 \sqrt{3} p_3, \\
p'_3 &= 6 \left( -2 p_2 + p_4^2 \right),
\end{aligned} \tag{79}$$

one obtains, for  $p'_4 = 1$ , the matrix  $R$  of class E2( $s = 1$ ), reported in II:

$$\begin{aligned}
R'_{11}(\tilde{p}') &= -4p'_1 + 5p'^2_2 + 5p'^2_3 + 12, \\
R'_{12}(\tilde{p}') &= 2p'_2(p'_3 + 3), \\
R'_{13}(\tilde{p}') &= p'^2_2 - p'_3(p'_3 - 6), \\
R'_{22}(\tilde{p}') &= p'_1 + 3p'_3 + 6, \\
R'_{23}(\tilde{p}') &= 3p'_2, \\
R'_{33}(\tilde{p}') &= p'_1 - 3p'_3 + 6.
\end{aligned} \tag{80}$$

### 3.12 Type $F_4$

The group is the group generated by all the reflections in  $\mathbb{R}^4$  which leave invariant the hyperplanes  $x_2 - x_3 = 0$ ,  $x_3 - x_4 = 0$ ,  $x_4 = 0$  and  $x_1 - x_2 - x_3 - x_4 = 0$ .

Let us define, for  $r = 2, 6, 8, 12$ :

$$\begin{aligned}
S_k(x) &= \sum_1^k x_i^k, \\
I_r(x) &= (8 - 2^{r-1})S_r + \sum_1^{r/2-1} j \binom{r}{2j} S_{2j} S_{r-2j} \\
&= \sum_{1 \leq i < j \leq 4} [(x_j + x_i)^r + (x_i - x_j)^r].
\end{aligned} \tag{81}$$

Then, according to Metha, a MIB for the group can be defined to be the following:

$$p_1(x) = I_{12}(x), \quad p_2(x) = I_8(x), \quad p_3(x) = I_6(x), \quad p_4(x) = I_2(x)/6, \tag{82}$$

or, explicitly:

$$\begin{aligned}
p_1(x) &= 924(x_1^6 + x_2^6 + x_3^6 + x_4^6)^2 + 990(x_1^4 + x_2^4 + x_3^4 + x_4^4)(x_1^8 + x_2^8 + x_3^8 + x_4^8) + 132(x_1^2 \\
&\quad + x_2^2 + x_3^2 + x_4^2)(x_1^{10} + x_2^{10} + x_3^{10} + x_4^{10}) - 2040(x_1^{12} + x_2^{12} + x_3^{12} + x_4^{12}), \\
p_2(x) &= 70(x_1^4 + x_2^4 + x_3^4 + x_4^4)^2 + 56(x_1^2 + x_2^2 + x_3^2 + x_4^2)(x_1^6 + x_2^6 + x_3^6 + x_4^6) - 120(x_1^8 \\
&\quad + x_2^8 + x_3^8 + x_4^8), \\
p_3(x) &= 30(x_1^2 + x_2^2 + x_3^2 + x_4^2)(x_1^4 + x_2^4 + x_3^4 + x_4^4) - 24(x_1^6 + x_2^6 + x_3^6 + x_4^6), \\
p_4(x) &= x_1^2 + x_2^2 + x_3^2 + x_4^2.
\end{aligned} \tag{83}$$

The essential elements of the associated  $\hat{P}(p)$  matrix turn out to be the following:

$$\begin{aligned}
\hat{P}_{11}(p) &= \left( 18711p_2^2p_3 + 1015740p_1p_2p_4 - 10178010p_2p_3^2p_4 - 625680p_1p_3p_4^2 + 12496p_3^3p_4^2 \right. \\
&\quad \left. - 1675080p_2^2p_4^3 - 5264820p_2p_3p_4^4 + 24793560p_1p_4^5 + 14410440p_3^2p_4^5 \right. \\
&\quad \left. - 254481480p_2p_4^7 + 470719260p_3p_4^8 - 1709728560p_4^{11} \right) / 810, \\
\hat{P}_{12}(p) &= 4 \left( 11970p_1p_3 - 610p_3^3 + 49977p_2^2p_4 - 175059p_2p_3p_4^2 + 428220p_1p_4^3 + 110052p_3^2p_4^3 \right. \\
&\quad \left. - 4455270p_2p_4^5 + 9531630p_3p_4^6 - 32435640p_4^9 \right) / 405, \\
\hat{P}_{13}(p) &= 4 \left( 243p_2^2 + 2259p_2p_3p_4 + 15480p_1p_4^2 - 5572p_3^2p_4^2 - 129240p_2p_4^4 + 278250p_3p_4^5 \right. \\
&\quad \left. - 847260p_4^8 \right) / 45, \\
\hat{P}_{22}(p) &= 16 \left( 21p_2p_3 + 84p_1p_4 - 28p_3^2p_4 - 840p_2p_4^3 + 1890p_3p_4^4 - 6120p_4^7 \right) / 3, \\
\hat{P}_{23}(p) &= 32 \left( 18p_1 + 7p_3^2 - 63p_2p_4^2 + 273p_3p_4^3 - 1134p_4^6 \right) / 9, \\
\hat{P}_{33}(p) &= 72 \left( -12 + p_2p_4 + 4p_3p_4^2 \right)
\end{aligned} \tag{84}$$

and, after the following MIBT:

$$\begin{aligned}
p'_1 &= 96\sqrt{6} \left( 288p_1 - 77p_3^2 - 3762p_2p_4^2 + 8832p_3p_4^3 - 29511p_4^6 \right) / 5, \\
p'_2 &= 108 \left( 16p_2 - 56p_3p_4 + 255p_4^4 \right) / 5, \\
p'_3 &= 6\sqrt{6} \left( 2p_3 - 15p_4^3 \right),
\end{aligned} \tag{85}$$

one obtains, for  $p'_4 = 1$ , the matrix  $R$  of class  $E4(s = 1)$ , reported in II:

$$\begin{aligned}
R'_{11}(\tilde{p}') &= -6 \left[ 12p'_1p'_3 - 21p'^2_2 - p'_2(11p'^2_3 - 864) - 36(17p'^2_3 + 972) \right], \\
R'_{12}(\tilde{p}') &= -6 \left[ 12p'_1 - p'_3(21p'_2 + p'^2_3 + 756) \right], \\
R'_{13}(\tilde{p}') &= p'^2_2 + 180p'_2 + 60p'^2_3, \\
R'_{22}(\tilde{p}') &= 6(9p'_2 + 7p'^2_3 + 972), \\
R'_{23}(\tilde{p}') &= p'_1 + 180p'_3, \\
R'_{33}(\tilde{p}') &= 5p'_2 + 324.
\end{aligned} \tag{86}$$

### 3.13 Type $H_4$

The group is defined as the group generated by all the reflections in  $\mathbb{R}^4$  which leave invariant the hyperplanes  $x_3 = 0$ ,  $x_4 = 0$ ,  $\tau^{-1}x_2 - \tau x_3 - x_4 = 0$  and  $\tau^{-1}x_1 - \tau x_2 - x_4 = 0$ , where  $\tau$  is defined in (63).

For  $j, k, l, m$  in the set  $\{1, 2, 3, 4\}$ , let us define the following symbols:

$$\eta_{jk} = \begin{cases} -1, & \text{for } j = k ; \\ 1, & \text{otherwise;} \end{cases} \quad (87)$$

and the following expressions:

$$\xi(m, j, k, l; x) = \tau x_j \eta_{mj} + \tau^{-1} x_k \eta_{mk} + x_l \eta_{ml}; \quad (88)$$

$$\chi(j, k, l, n; x) = \xi(0, j, k, l; x)^{2n} + \xi(j, j, k, l; x)^{2n} + \xi(k, j, k, l; x)^{2n} + \xi(l, j, k, l; x)^{2n}; \quad (89)$$

$$\psi(j, n; x) = \left( \sum_1^4 \eta_{jk} x_k \right)^{2n}. \quad (90)$$

$$\begin{aligned} I_n(x) = & \sum_1^4 (2x_k)^{2n} + \sum_0^4 \psi(k; x) + \chi(1, 2, 3, n; x) + \chi(1, 3, 4, n; x) \\ & + \chi(1, 4, 2, n; x) + \chi(2, 4, 3, n; x). \end{aligned} \quad (91)$$

Then, according to Metha, a MIB for  $H_4$  can be chosen in the following way:

$$p_1(x) = I_{30}(x), \quad p_2(x) = I_{20}(x), \quad p_3(x) = I_{12}(x), \quad p_4(x) = \sum_1^4 x_i^2. \quad (92)$$

The essential elements of the associated  $\hat{P}$ -matrix turn out to be the following:

$$\begin{aligned} \hat{P}_{11}(p) = & 53911 p_2 p_3^3 p_4 / 7616 + 7051785 p_1 p_3^2 p_4^2 / 56 + 4821334245 p_2^2 p_3 p_4^3 / 25432 \\ & + 2186873325 p_1 p_2 p_4^4 / 34 - 645826368707 p_3^4 p_4^5 / 150528 \\ & - 116309076672555 p_2 p_3^2 p_4^7 / 23936 - 211651127025 p_1 p_3 p_4^8 / 2 \\ & - 21238646708813625 p_2^2 p_4^9 / 18496 - 283066493617380915 p_3^3 p_4^{11} / 9856 \\ & - 2811241304150172075 p_2 p_3 p_4^{13} / 544 + 2218140033302250 p_1 p_4^{14} \\ & + 7676790020731375739325 p_3^2 p_4^{17} / 224 - 15228773425368084479625 p_2 p_4^{19} / 136 \\ & + 253639342346876415408375 p_3 p_4^{23} / 8 \\ & - 8927280781972196041680013125 p_4^{29} / 4, \\ \hat{P}_{12}(p) = & 26741 p_3^4 / 61740 + 2357459 p_2 p_3^2 p_4^2 / 56 + 1473900 p_1 p_3 p_4^3 + 482714505 p_2^2 p_4^4 / 22 \\ & - 1869793842241 p_3^3 p_4^6 / 7056 - 7474081897815 p_2 p_3 p_4^8 / 44 \\ & + 327790212400 p_1 p_4^9 + 66300758108151125 p_3^2 p_4^{12} / 308 \\ & - 34964650402339275 p_2 p_4^{14} + 128303960304363056775 p_3 p_4^{18} \\ & - 993168612785995074523500 p_4^{24}, \\ \hat{P}_{13}(p) = & 429975 p_2^2 / 3179 + 4236791 p_3^3 p_4^2 / 168 + 2490103980 p_2 p_3 p_4^4 / 187 \end{aligned}$$

$$\begin{aligned}
& +92563800p_1p_4^5 - 7157961621135p_3^2p_4^8/88 - 330008206170825p_2p_4^{10}/34 \\
& +36082213228297575p_3p_4^{14} - 271058613666147798750p_4^{20}, \\
\hat{P}_{22}(p) = & 2657644p_3^3p_4/138915 + 24894256p_2p_3p_4^3/21 + 5074562560p_1p_4^4/819 \\
& -1343036354024p_3^2p_4^7/441 - 644361278880p_2p_4^9 \\
& +49357102179756800p_3p_4^{13}/21 - 4855838749013355171200p_4^{19}/273, \\
\hat{P}_{23}(p) = & 10880p_1/13 + 1322362p_3^2p_4^3/21 - 80135160p_2p_4^5 + 296137692080p_3p_4^9 \\
& -29473265236173600p_4^{15}/13, \\
\hat{P}_{33}(p) = & 5040p_4(7p_2 - 18224p_3p_4^4 + 167747160p_4^{10})/17
\end{aligned} \tag{93}$$

and, after the following MIBT:

$$\begin{aligned}
p'_1 = & 98415000 \left( 576p_1/1001 - 108555p_3^2p_4^3/539 - 11535372p_2p_4^5/187 \right. \\
& \left. +17469633928p_3p_4^9/77 - 1724135397013808p_4^{15}/1001 \right), \\
p'_2 = & 2187000 \left( -6p_2/187 + 1307p_3p_4^4/11 - 908706p_4^{10} \right), \\
p'_3 = & 1620 \left( -p_3/7 + 1130p_4^6 \right).
\end{aligned} \tag{94}$$

one obtains, for  $p'_4 = 1$ , the matrix  $R$  of class  $E5(s=1)$  reported in  $\Pi^6$ :

$$\begin{aligned}
\hat{R}'_{11}(p') = & -36p_2^2(-25380 + 19p_3) + 90p_1(-1166400 + 12p_2 + 1080p_3 + p_3^2) \\
& -p_2(-75582720000 - 342921600p_3 - 6480p_3^2 + 29p_3^3) \\
& +45(918330048000000 + 906992640000p_3 + 1102248000p_3^2 \\
& -339120p_3^3 + 209p_3^4), \\
\hat{R}'_{12}(p') = & -486p_2^2 + 360p_1(540 + p_3) - 9p_2(-34992000 - 3240p_3 + 19p_3^2) \\
& -p_3(-89754480000 + 28431000p_3 - 45360p_3^2 + p_3^3), \\
\hat{R}'_{13}(p') = & 2160p_1 + p_2^2 - 1980p_2(-1080 + p_3) - 55(-4860 + p_3)p_3^2, \\
\hat{R}'_{22}(p') = & 212576400000 + 540p_1 - 45927000p_3 + 218700p_3^2 - 19p_3^3 - 324p_2(2025 + p_3), \\
\hat{R}'_{23}(p') = & p_1 - 810p_2 - 495(-2700 + p_3)p_3, \\
\hat{R}'_{33}(p') = & 11p_2 - 6750(-1296 + p_3).
\end{aligned} \tag{95}$$

## 4 Reducible reflection groups with 2, 3 and 4 basic invariants

In this section we shall state the rules for building the  $\hat{P}$ -matrices of a reducible coregular linear group  $G$ , in a standard A-basis, starting from the  $\hat{P}$ -matrices associated to its irreducible components. This will allow us, in particular, to derive the explicit form of the  $\hat{P}$ -matrices

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<sup>6</sup>In  $\Pi$ , the sign of the monomial  $p_1p_3$  in the expression of  $R'_{11}$  is wrong and should be changed; accordingly should be changed the expression of  $A(p)$ .

of all the reducible reflection groups whose orbit spaces have dimensions  $\leq 4$  and state which of the allowable  $\hat{P}$ -matrices determined in I and II are related to these groups.

Let  $G^{(1)}$  and  $G^{(2)}$  be irreducible CLG's, acting, respectively, in  $\mathbb{R}^{n_1}$  and  $\mathbb{R}^{n_2}$ . Then, the set of matrices

$$G = \{g^{(1)} \oplus g^{(2)}\}_{g^{(\alpha)} \in G^{(\alpha)} \atop \alpha=1,2} \quad (96)$$

forms a coregular linear group, acting on the vectors  $x = x^{(1)} \oplus x^{(2)}$ ,  $x \in \mathbb{R}^{n_1+n_2} = \mathbb{R}^{n_1} \oplus \mathbb{R}^{n_2}$ . If the groups  $G^{(\alpha)}$ ,  $\alpha = 1, 2$  are generated by reflections,  $G$  is a reflection group isomorphic to  $G_1 \otimes G_2$ .

Let us denote by  $p_i^{(\alpha)}(x^{(\alpha)})$ ,  $i = 1, \dots, q_\alpha$ ,  $x^{(\alpha)} \in \mathbb{R}^{n_\alpha}$  the elements of a standard MIB relative to  $G^{(\alpha)}$ ,  $\alpha = 1, 2$  and by  $\{d_i^{(\alpha)}\}$ ,  $\hat{P}^{(\alpha)}(p^{(\alpha)})$  the associated set of degrees and  $\hat{P}$ -matrix. We shall assume  $d_1^{(1)} \geq d_1^{(2)}$ .

A set of basic polynomial invariants of  $G$  is yielded by

$$p^{(+)}(x) = \{p^{(1)}(x^{(1)}), p^{(2)}(x^{(2)})\}. \quad (97)$$

and the associated  $\hat{P}$ -matrix has the following form:

$$\hat{P}^{(+)}(p^{(+)}) = \hat{P}^{(1)}(p^{(1)}) \oplus \hat{P}^{(2)}(p^{(2)}). \quad (98)$$

If  $\{p^{(\alpha)}\}$  is a standard  $A$ -basis relative to  $G^{(\alpha)}$ ,  $A^{(\alpha)}(p^{(\alpha)})$  is the complete active factor of  $\det \hat{P}^{(\alpha)}(p^{(\alpha)})$  and  $w^{(\alpha)}$  is its weight, then

$$A^{(+)}(p^{(+)}) = A^{(1)}(p^{(1)}) A^{(2)}(p^{(2)}) \quad (99)$$

is the complete active factor of  $\det \hat{P}^{(+)}$ ; it satisfies the following relations:

$$\sum_1^{q_1+q_2} b \hat{P}_{ab}^{(+)}(p^{(+)}) \partial_b A^{(+)}(p^{(+)}) = \lambda_a^{(+)} A^{(+)}(p^{(+)}) , \quad a = 1, \dots, q_1 + q_2 , \quad (100)$$

where

$$\lambda^{(+)} = \lambda^{(1)} \oplus \lambda^{(2)} = (0, \dots, 0, 2w^{(1)}, 0, \dots, 0, 2w^{(2)}). \quad (101)$$

Therefore, a standard  $A$ -basis  $\{p\}$  of  $G$  can be obtained from  $\{p^{(+)}\}$  by means of a basis transformation  $p = f(p^{(+)})$ , with  $f(p^{(+)})$  defined, for instance, by the following relations:

$$\begin{aligned} p_k &= p_{i(k)}^{(+)}, & k &= 1, \dots, q_1 + q_2 - 2, \\ p_{q_1+q_2-1} &= b_{q_1+q_2-1} \left( w^{(2)} p_{q_1}^{(1)} - w^{(1)} p_{q_2}^{(2)} \right), \\ p_{q_1+q_2} &= p_{q_1}^{(1)} + p_{q_2}^{(2)}; \end{aligned} \quad (102)$$

in (102), the set  $\{i(1), \dots, i(q_1 + q_2 - 2)\}$  is a permutation of the indices  $\{1, \dots, q_1 + q_2 - 2\}$ , such that the degrees of the invariants  $p_k$  are non increasing functions of  $k$ . The parameters

$b_k$  are arbitrary and will be chosen so that the  $\hat{P}$ -matrices can be easily compared with the results reported in I and II.

The  $\hat{P}$ -matrix associated to the MIB  $\{p\}$  is determined by the following relation (see (15)):

$$\hat{P}(p) = J(p^{(+)}) \hat{P}^{(+)}(p^{(+)}) J^T(p^{(+)}) \Big|_{p^{(+)} = f^{-1}(p)}, \quad (103)$$

where  $J(p^{(+)})$  denotes the Jacobian matrix

$$J_{ab}(p^{(+)}) = \frac{\partial f_a(p^{(+)})}{\partial p_b^{(+)}}, \quad a, b = 1, \dots, q_1 + q_2. \quad (104)$$

In the aim of determining the  $\hat{P}$ -matrices of all the reducible reflection groups whose orbit spaces have dimensions 3 and 4, let us now specialize the construction we have described to the cases  $q_1 = 2$ ,  $q_2 = 1, 2$  and to each of the different cases one can get starting from  $q_1 = 3$ ,  $q_2 = 1$ . We shall denote by  $w$  the weight of the complete active factor  $A(p)$  of  $\det \hat{P}(p)$ :

$$w = w^{(+)} = w^{(1)} + w^{(2)}. \quad (105)$$

Below, for each of the different reducible groups that can be obtained in this way, we shall list the values of the degrees, the explicit form of the matrix  $R^{(+)}$ , the MIBT leading to a standard  $A$ -basis and the transformed form of the matrix  $R(p)$ , evaluated at  $p_q = 1$ , to be compared with the results of I and II.

#### 4.1 Case $q_1 = 2$ , $q_2 = 1$

$$\begin{aligned} d_1 &= d_1^{(1)} = m + 1, & d_3 &= d_1^{(2)} = 2, & m &\in \mathbb{N}_*; \\ d_2 &= d_2^{(1)} = 2, & w &= 2d_1^{(1)} + 2 = 2m + 4; \end{aligned} \quad (106)$$

$$\begin{aligned} R_{11}^{(+)}(p^{(+)}) &= p_2^{(1)m}, & R_{a3}^{(+)}(p^{(+)}) &= 0, & a &= 1, 2, \\ R_{12}^{(+)}(p^{(+)}) &= p_1^{(1)}, & R_{33}^{(+)}(p^{(+)}) &= p_1^{(2)}, \\ R_{22}^{(+)}(p^{(+)}) &= p_2^{(1)}, & R_{44}^{(+)}(p^{(+)}) &= p_2^{(2)}; \end{aligned} \quad (107)$$

$$\begin{aligned} p_1 &= (2 + m)^{m/2} p_1^{(1)}, \\ p_2 &= -p_2^{(1)} + (m + 1)p_1^{(2)}, \\ p_3 &= p_2^{(1)} + p_1^{(2)}; \end{aligned} \quad (108)$$

$$\begin{aligned} R_{11}(p) &= [(1 + m)p_3 - p_2]^m, & R_{22}(p) &= (1 + m)p_3 + mp_2, \\ R_{12}(p) &= -p_1; & R_{a3}(p) &= p_a, & a &= 1, 2, 3; \end{aligned} \quad (109)$$

which, for  $p_3 = 1$ , is the class II  $R$ -matrix reported in II.

## 4.2 Case $q_1 = 2, q_2 = 2$

$$\begin{aligned} d_1 = d_1^{(1)} = j_1 + 1, \quad d_3 = d_2^{(1)} = 2, \quad j_1, j_2 \in \mathbb{N}_*; \\ d_2 = d_1^{(2)} = j_2 + 1, \quad d_4 = d_2^{(2)} = 2, \end{aligned} \quad (110)$$

$$w = w^{(1)} + w^{(2)} = 2(j_1 + j_2 + 2); \quad (111)$$

$$\begin{aligned} R_{11}^{(+)}(p^{(+)}) &= p_2^{(1)j_1}, & R_{22}^{(+)}(p^{(+)}) &= p_2^{(1)}, & R_{34}^{(+)}(p^{(+)}) &= p_1^{(2)}, \\ R_{12}^{(+)}(p^{(+)}) &= p_1^{(1)}, & R_{33}^{(+)}(p^{(+)}) &= p_2^{(2)j_2}, & R_{44}^{(+)}(p^{(+)}) &= p_2^{(2)}; \\ R_{ab}^{(+)}(p^{(+)}) &= 0, & a &= 1, 2, & b &= 3, 4; \end{aligned} \quad (112)$$

$$\begin{aligned} p_1 &= (j_1 + j_2 + 2)^{\frac{j_1}{2}} p_1^{(1)}, & p_3 &= (j_2 + 1)p_2 - (j_1 + 1)p_4, \\ p_2 &= (j_1 + j_2 + 2)^{\frac{j_1}{2}} p_1^{(2)}, & p_4 &= p_2^{(1)} + p_2^{(2)}; \end{aligned} \quad (113)$$

$$\begin{aligned} R_{11}(p) &= (j_1 + j_2 + 2)[-p_3 + (j_1 + 1)p_4]^{j_1}, & R_{12}(p) &= 0, \\ R_{22}(p) &= (j_1 + j_2 + 2)[p_3 + (j_2 + 1)p_4]^{j_2}, & R_{13}(p) &= -(j_2 + 1)p_1, \\ R_{33}(p) &= (j_1 + 1)(j_2 + 1) + (j_1 - j_2)p_3, & R_{23}(p) &= (j_1 + 1)p_2, \end{aligned} \quad (114)$$

which, for  $p_3 = 1$ , is the class  $A8(j_1, j_2)$   $R$ -matrix reported in II. For  $j_i = 1$  the group  $G^{(i)} \simeq Z_2 \otimes Z_2$  is reducible.

## 4.3 Cases $q_1 = 3, q_2 = 1$

$$\begin{aligned} d_1 &= d_1^{(1)}, & d_3 &= d_3^{(1)}, & w &= w^{(1)} + 2; \\ d_2 &= d_2^{(1)}, & d_4 &= d_1^{(2)}, \end{aligned} \quad (115)$$

$$\begin{aligned} R^{(+)}(p^{(+)})_{ab} &= R_{ab}^{(1)}(p^{(1)}), & a, b &= 1, 2, 3, \\ R^{(+)}(p^{(+)})_{a4} &= 0, & a &= 1, 2, 3, \\ R^{(+)}(p^{(+)})_{44} &= R_{11}^{(2)}(p^{(2)}) = p_1^{(2)}; \end{aligned} \quad (116)$$

$$\begin{aligned} p_1 &= b_1 p_1^{(1)}, & p_3 &= b_3 \left( p_3^{(1)} - w^{(1)} p_1^{(2)} / 2 \right), \\ p_2 &= b_2 p_2^{(1)}, & p_4 &= p_3^{(1)} + p_1^{(2)}. \end{aligned} \quad (117)$$

The matrix  $R^{(1)}$  can be chosen from 3 different classes, denoted as III.1, III.2, III.3 in II and corresponding, respectively, to the groups of type  $A_3$  (or  $D_3$ ),  $B_3$  and  $H_3$ .

Choosing as  $G^{(1)}$  a type  $A_3$  group one obtains:

$$\begin{aligned} d_1 &= 4, & d_3 &= d_4 = 2, \\ d_2 &= 3, & w^{(1)} &= 12; \end{aligned} \quad (118)$$

$$\begin{aligned} p_1 &= 49p_1^{(1)}, & p_3 &= p_3^{(1)} - 6p_1^{(2)}, \\ p_2 &= -7^{\frac{3}{2}}p_2^{(1)}; & p_4 &= p_3^{(1)} + p_1^{(2)}; \end{aligned} \quad (119)$$

$$\begin{aligned} R_{11}(p) &= 7 \left[ p_2^2 - p_1(p_3 + 6p_4) + 2(p_3 + 6p_4)^3 \right], \\ R_{22}(p) &= 7 \left[ p_1 + 2(p_3 + 6p_4)^2 \right], \\ R_{12}(p) &= 14p_2(p_3 + 6p_4), \\ R_{13}(p) &= p_1, & R_{23}(p) &= p_2, & R_{33}(p) &= -5p_3 + 6p_4, \end{aligned} \quad (120)$$

which, for  $p_4 = 1$ , is the class B4( $s = 1$ )  $R$ -matrix reported in II.

Choosing as  $G^{(1)}$  a type B<sub>3</sub> group one obtains:

$$\begin{aligned} d_1 &= 6, & d_3 &= d_4 = 2, \\ d_2 &= 4, & w^{(1)} &= 18; \end{aligned} \quad (121)$$

$$\begin{aligned} p_1 &= 10^3 p_1^{(1)}, & p_3 &= p_3^{(1)} - 9p_1^{(2)}, \\ p_2 &= -10^2 p_2^{(1)}, & p_4 &= p_3^{(1)} + p_1^{(2)}; \end{aligned} \quad (122)$$

$$\begin{aligned} R_{11}(p) &= 10 \left\{ p_1 \left[ p_2 - 4(p_3 + 9p_4)^2 \right] + 8(p_3 + 9p_4) \left[ p_2^2 \right. \right. \\ &\quad \left. \left. + 2p_2(p_3 + 9p_4)^2 + 8(p_3 + 9p_4)^4 \right] \right\}, \\ R_{12}(p) &= 10 \left\{ 2p_1(p_3 + 9p_4) - p_2 \left[ p_2 - 12(p_3 + 9p_4)^2 \right] \right\}, \\ R_{22}(p) &= 10 \left\{ p_1 - 4(p_3 + 9p_4) \left[ p_2 - 4(p_3 + 9p_4)^2 \right] \right\}, \\ R_{13}(p) &= p_1, & R_{23}(p) &= p_2, & R_{33}(p) &= -8p_3 + 9p_4, \end{aligned} \quad (123)$$

which, for  $p_4 = 1$ , is the class C6(1)  $R$ -matrix reported in II.

Choosing as  $G^{(1)}$  a type H<sub>3</sub> group one obtains:

$$\begin{aligned} d_1 &= 10, & d_3 &= d_4 = 2, \\ d_2 &= 6, & w^{(1)} &= 30, \end{aligned} \quad (124)$$

$$\begin{aligned} p_1 &= 16^5 p_1^{(1)}, & p_3 &= p_3^{(1)} - 15p_1^{(2)}, \\ p_2 &= -16^3 p_2^{(1)}, & p_4 &= p_3^{(1)} + p_1^{(2)}; \end{aligned} \quad (125)$$

$$R_{11}(p) = 16 \left\{ 4p_1(p_3 + 15p_4) \left[ p_2 - 3(p_3 + 15p_4)^3 \right] - [p_2 - 48(p_3 + 15p_4)^3] \left[ p_2^2 + 4p_2(p_3 + 15p_4)^3 + 24(p_3 + 15p_4)^6 \right] \right\}, \quad (126)$$

$$\begin{aligned} R_{12}(p) &= 16(p_3 + 15p_4) \left[ -5p_2^2 + 6p_1(p_3 + 15p_4) + 60p_2(p_3 + 15p_4)^3 \right], \\ R_{22}(p) &= 16 \left[ p_1 - 14p_2(p_3 + 15p_4)^2 + 96(p_3 + 15p_4)^5 \right], \\ R_{13}(p) &= p_1, \quad R_{23}(p) = p_2, \quad R_{33}(p) = -14p_3 + 15p_4, \end{aligned} \quad (127)$$

which, for  $p_4 = 1$ , is the class  $D4(j_1)$   $R$ -matrix reported in II.

## 5 Concluding remarks on the mathematical results

Starting from explicit forms for the basic polynomial invariants of the finite coregular groups, that can be found in the mathematical literature, we have computed the associated  $\hat{P}(p)$  matrices. The equalities and inequalities, defining the orbit spaces of the groups as semi-algebraic sub-varieties of  $\mathbb{R}^q$ , can be easily obtained as semi-positivity conditions on these matrices.

The computation has been limited to the groups with less than 5 basic polynomial invariants, since the main aim of our work was to test the completeness of the allowable solutions of the canonical equation listed in I and II and to find the corresponding generating groups. The test has been positive: all the  $\hat{P}$ -matrices generated by finite coregular groups appear in the lists of allowable  $\hat{P}$ -matrices reported in I and II. In particular:

1. For  $q = 2$  all the allowable  $\hat{P}$ -matrices are generated by coregular *finite* groups; the case  $q = 2$  is exceptional, since the canonical equation puts no restrictions on the allowable  $\hat{P}$ -matrices. On the contrary, for  $q = 3, 4$ , only the fundamental elements (scale parameter  $s = 1$ ) of some towers of allowable  $\hat{P}$ -matrices are generated by coregular *finite* groups; in this case, the existence of towers of solutions of the canonical equation has probably no group theoretical meaning, but is only an artifact related to an invariance of the canonical equation under scaling of the degrees of the basic polynomial invariants. By now, we cannot exclude however that the higher elements in the towers are generated by non-finite groups.
2. For  $q = 2, 3, 4$  all the *fully active* allowable solutions of the canonical equation are generated by *finite* coregular linear groups; the *irreducible* ones are associated to *irreducible* linear groups.

As for the fundamental allowable  $\hat{P}$ -matrices for which we have not found a finite coregular generating group, various, more or less obvious, interpretations are possible; they might be generated by

- i) non-finite compact coregular groups,

- ii) non-coregular groups,
- iii) non-minimal integrity bases of finite or non-finite compact coregular groups,
- iv) direct sums of non-fundamental allowable  $\hat{P}$ -matrices.

This is probably an incomplete list.

We shall try to clarify this point in two forthcoming papers. The correspondence between the classification of the allowable  $\hat{P}$ -matrices determined in I and II and the generating finite reflection groups with less than 5 basic polynomial invariants is summarized in Tables 1-4, where by a group of type  $I_2(1)$  we mean the group  $Z_2 \otimes Z_2$ , ( $Z_2 = \{\pm 1\}$ ). The case  $q = 1$  is trivial, as there is only one allowable  $\hat{P}$ -matrix generated by the group  $Z_2$ . For  $q = 2$ , for each choice of the degree  $d_1$  there is only one equivalence class of allowable  $\hat{P}$ -matrices, which are generated by at least one finite coregular linear group. For  $q = 3$ , all the fundamental elements in each tower of (classes of) allowable solutions are generated by at least one finite coregular group, but for the  $\hat{P}$ -matrices of class I. For  $q = 4$ , the number of (classes of) reducible allowable solutions which are not generated by at least one finite coregular group is much higher.

## 6 Physical applications. An example

The  $\hat{P}$  matrix approach to the study of orbit spaces has been, or can be used, in various physical contexts, where the study of covariant functions is important, as already stressed in the introduction. Typical examples are the determination of patterns of spontaneous symmetry and/or supersymmetry breaking [20, 7] in gauge field theories of elementary particles, the analysis of phase spaces and structural phase transitions in the framework of Landau's theory [49, 50] and in cosmology (phase transitions in the hot Universe [51]). Applications can be done in covariant bifurcation theory [52] or in crystal field theory and in most areas of solid state theory where use is made of symmetry adapted functions.

Most of the groups dealt with in the preceding sections are crystallographic groups, they are therefore symmetry groups of regular polyhedra in 2, 3 or 4 dimensions and of root diagrams of simple Lie algebras. In particular,  $I_2(m)$  denotes, in Coxeter's notation, the dihedral group denoted by  $C_{nv}$  in the standard physical notation [49],  $I_2(m) \otimes \mathbb{Z}_2$  denotes  $D_{nh}$ , while  $D_3$ ,  $B_3$  and  $H_3$  correspond, respectively, to the groups  $T_d$ ,  $O_h$  and  $Y_h$ ;  $F_4$  is the symmetry group of a regular solid in  $\mathbb{R}^4$  with 24 3-dimensional octahedral faces;  $H_4$  is the symmetry group of a regular solid in  $\mathbb{R}^4$  with 120 3-dimensional dodecahedral faces or, dually, of a regular 600-sided solid with tetrahedral faces; the groups  $A_3$ ,  $A_4$ ,  $B_4$  and  $D_4$  are strictly related to permutation groups or semi-direct products of permutation groups and sign change groups, as explained in §3.

Solid state physics is, therefore, a natural physical context where our results can be exploited. As an example of the use of the  $\hat{P}$ -matrix approach to the analysis of properties of an invariant function, and in particular of the determination of the location of its stationary points and of its absolute minimum, in this section we shall study a six-degree expansion

of a Landau thermodynamic potential  $G(x; \pi, T)$ , which depends on the vector valued order parameter  $x = (x_1, x_2, x_3)$ , transforming according to the fundamental representation of the group  $O_h$ . At the end we shall specialize our results to BaTiO<sub>3</sub> and determine its phase space using an oversimplified expression for its free-energy.

### 6.1 The orbit space of the group $O_h$ and its stratification

In the Coxeter notations used in the preceding sections, the fundamental representation of the group  $O_h$  corresponds to the group  $B_3$ , for which a MIB is specified in (56) and the corresponding  $\hat{P}$ -matrix in (57) and (13), with  $d_1 = 6$ ,  $d_2 = 4$ ,  $d_3 = 2$ .

To describe the geometry of the image  $\bar{\mathcal{S}}$  of the orbit space of  $O_h$ , let us define the following auxiliary polynomial functions of  $p$ :

$$\begin{aligned} f_1(p) &= -p_2 + p_3^2, \\ f_2(p) &= -p_1 + p_3^3, \\ f_3(p) &= 3p_2 - p_3^2, \\ f_4(p) &= 9p_1 - p_3^3, \\ f_5(p) &= 2p_2 - p_3^2, \\ f_6(p) &= 4p_1 - p_3^3, \\ f_7(p) &= p_3^3 - 3p_3p_2 + 2p_1, \\ f_8(p) &= -p_3^6 + 9p_2p_3^4 - 8p_1p_3^3 - 21p_2^2p_3^2 + 36p_1p_2p_3 + 3p_2^3 - 18p_1^2. \end{aligned} \quad (128)$$

The shape and primary stratification of  $\bar{\mathcal{S}}$  can be immediately deduced from an inspection of the condition

$$\det \hat{P}(p) = f_7(p)f_8(p) = 0; \quad (129)$$

the results obtained in this way are confirmed by a complete analysis of the positivity and rank conditions on the matrix  $\hat{P}(p)$  defined in (57). The section  $\Xi$  of the orbit space with the plane  $p_3 = \text{const}$  is plotted in figure 1, where the axes are labelled by the adimensional variables

$$u = p_2/p_3^2, \quad v = p_1/p_3^3. \quad (130)$$

The determination of the isotropy type stratification of  $\bar{\mathcal{S}}$ , that is the determination of the orbit types of the different primary strata, requires a sounder analysis: for a convenient choice of the point  $\bar{p}$  in each stratum, one has first to find a solution  $\bar{x} = (\bar{x}_1, \bar{x}_2, \bar{x}_3)$  of the following equations<sup>7</sup>:

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<sup>7</sup>The numbers  $(\bar{x}_1, \bar{x}_2, \bar{x}_3)$  are the non-negative solutions of the real equation  $\sum_{k=0}^3 a_k z^k = 0$ , with  $a_0 = (-\bar{p}_3^3 + 2\bar{p}_2\bar{p}_3 - 2\bar{p}_1)/6$  ( $= -\bar{x}_1^2\bar{x}_2^2\bar{x}_3^2$ ),  $a_1 = (\bar{p}_3^2 - \bar{p}_2)/2$  ( $= \bar{x}_1^2\bar{x}_2^2 + \bar{x}_2^2\bar{x}_3^2 + \bar{x}_3^2\bar{x}_1^2$ ),  $a_2 = \bar{p}_3$  ( $= \bar{x}_1^2 + \bar{x}_2^2 + \bar{x}_3^2$ ),  $a_3 = 1$ .

$$\begin{cases} x_1^6 + x_2^6 + x_3^6 &= \bar{p}_1, \\ x_1^4 + x_2^4 + x_3^4 &= \bar{p}_2, \\ x_1^2 + x_2^2 + x_3^2 &= \bar{p}_3, \end{cases} \quad (131)$$

and then, to determine the isotropy subgroup of  $O_h$  at  $\bar{x}$ , by selecting the transformations of  $O_h$  which leave  $\bar{x}$  invariant.

A solution  $\bar{x}$  of (131) for each stratum is easily found by noting that

$$\begin{aligned} \det \hat{P}(p(x)) &= f_7(p(x))f_8(p(x)) \\ &= 36x_1^2x_2^2x_3^2(x_1^2 - x_2^2)^2(x_2^2 - x_3^2)^2(x_3^2 - x_1^2)^2. \end{aligned} \quad (132)$$

The results one obtains are reported in table 5.

## 6.2 The absolute minimum of the potential. Phase transitions

Let us now build the potential

$$G(x; \pi, T) = \hat{G}(p(x); \pi, T), \quad (133)$$

as the most general sixth order  $O_h$  invariant polynomial function of the order parameters, the coefficients  $c, A_i$  and  $B_j$  being functions of the pressure  $\pi$  and the absolute temperature  $T$ :

$$\hat{G}(p; \pi, T) = \frac{c}{2}p_3 + \frac{1}{4}(A_0p_3^2 + A_1p_2) + \frac{1}{6}(B_0p_3^3 + B_1p_3p_2 + B_2p_1). \quad (134)$$

In order to assure stability of the system, we shall require that  $G(x; \pi, T)$  is bounded below. This occurs if and only if the coefficient of  $p_3^3$  in the asymptotic form of  $\hat{G}$  for  $p_3 \rightarrow \infty$ :

$$C_{as}(u, v) = \frac{1}{6}(B_0 + B_1u + B_2v) \quad (135)$$

is everywhere positive on  $\Xi$ , i.e. iff its minimum in  $\Xi$  is  $> 0$ . Since the equation  $C_{as}(u, v) = \text{const}$  defines straight lines in the plane  $(u, v)$  and  $\bar{\mathcal{S}}$  is inscribed in a triangle with vertices at the points representing the strata  $\{C_{iv}\}$ ,  $i = 2, 3, 4$  (see figure 1), one easily realizes that  $C_{as}(u, v)$  is bound to take on its absolute minimum at at least one of the vertices. Therefore,  $\hat{G}(p; \pi, T)$  is bounded below if and only if the following inequalities are satisfied:

$$\begin{cases} C_{as}(u, v)|_{\{C_{2v}\}} &= (4B_0 + 2B_1 + B_2)/4 > 0, \\ C_{as}(u, v)|_{\{C_{3v}\}} &= (9B_0 + 3B_1 + B_2)/9 > 0, \\ C_{as}(u, v)|_{\{C_{4v}\}} &= B_0 + B_1 + B_2 > 0. \end{cases} \quad (136)$$

Being  $\hat{G}(p; \pi, T)$  a linear function of  $(p_1, p_2)$ , for fixed  $p_3$ , the extremal points of  $\hat{G}(p; \pi, T)$  lie necessarily on the boudary of  $\bar{\mathcal{S}}$  and can be determined [21] using, for instance, the standard

method of Lagrange multipliers. Denoting by  $f_A = 0$ ,  $A \in \mathcal{I}_\alpha^{(0)}$  and  $f_A > 0$ ,  $A \in \mathcal{I}_\alpha^{(+)}$  the algebraic relations defining the isotropy stratum  $\Sigma_\alpha$ , the conditions one obtains can be written in the following form:

$$\begin{cases} \frac{\partial \widehat{G}}{\partial p_a} = \sum_{A \in \mathcal{I}_\alpha^{(0)}} \lambda_A \frac{\partial f_A}{\partial p_A}, & a = 1, 2, \dots, q, \\ f_A = 0 & A \in \mathcal{I}_\alpha^{(0)}, \\ f_A > 0, & A \in \mathcal{I}_\alpha^{(+)}, \end{cases} \quad (137)$$

where the  $\lambda$ 's are Lagrange multipliers.

The determination of the absolute minimum and of its location(s) is made much easier if one notes that  $\widehat{G}(p; \pi, T)$  necessarily takes on its absolute minimum in some point of one of the strata  $\{\mathcal{O}_h\}$ ,  $\{\mathcal{C}_{iv}\}$ ,  $i = 2, 3, 4$ <sup>8</sup>, like  $C_{as}(u, v)$  and for the same reasons.

By indexing these strata in the following way:

$$\Sigma_0 = \{\mathcal{O}_h\}, \quad \Sigma_1 = \{\mathcal{C}_{4v}\}, \quad \Sigma_2 = \{\mathcal{C}_{2v}\}, \quad \Sigma_3 = \{\mathcal{C}_{3v}\}, \quad (138)$$

the relations determining the stationary points of the potential can be put in a very compact form.

The relations defining the strata  $\Sigma_k$ , which can be read from table 5, allow to express  $p_1$  and  $p_2$  in terms of  $p_3$ , so that we can define

$$\widehat{G}_k(p_3; \pi, T) = \widehat{G}(p; \pi, T)|_{\Sigma_k}, \quad k = 0, \dots, 3. \quad (139)$$

Explicitly:

$$\widehat{G}_0(0; \pi, T) = 0, \quad (140)$$

$$\widehat{G}_k(p_3; \pi, T) = p_3 \left( \frac{c}{2} + \frac{a_k p_3}{4} + \frac{b_k p_3^2}{6} \right), \quad p_3 > 0, \quad (141)$$

where

$$\begin{aligned} a_k &= A_0 + A_1 k^{-1}, \\ b_k &= B_0 + B_1 k^{-1} + B_2 k^{-2}, \end{aligned} \quad k = 1, 2, 3, \quad (142)$$

and, owing to (136),  $b_k > 0$ .

Now, it is trivial to realize that for  $c < 0$ , each of the functions  $\widehat{G}_k(p_3; \pi, T)$ ,  $k = 1, 2, 3$  has a local minimum, which is unique and is located at  $p_3 = p_{3,k}$ , where

$$p_{3,k} = \frac{\left( -a_k + \sqrt{a_k^2 - 4b_k c} \right)}{2b_k}. \quad (143)$$

---

<sup>8</sup>The possibility of a degenerate minimum crossing the strata  $\{\mathcal{C}_{2v}\}$ ,  $\{\mathcal{C}'_s\}$  and  $\{\mathcal{C}_{4v}\}$  can be excluded by a direct check.

At  $p_3 = p_{3,k}$ , the function  $\hat{G}_k(p_3; \pi, T)$  takes on the value:

$$\hat{G}_k^{\min}(\pi, T) = \frac{1}{48b_k^2} \left( a_k - \sqrt{a_k^2 - 4b_k c} \right) \left( a_k^2 - 8b_k c - a_k \sqrt{a_k^2 - 4b_k c} \right), \quad k = 1, 2, 3. \quad (144)$$

For  $c \geq 0$ , only  $\hat{G}_1(p_3; \pi, T)$  has a local minimum, which is unique and is located at  $p_3 = p_{3,1}$ , with  $p_{3,1}$  defined in (143) and  $\hat{G}_1^{\min}(\pi, T)$  defined in (144).

To determine the absolute minimum of  $\hat{G}(p; \pi, T)$  and the phase space, it remains only to compare the values taken on by the functions  $\hat{G}_k^{\min}(\pi, T)$ ,  $k = 0, \dots, 3$ , for  $c < 0$  and the functions  $\hat{G}_1^{\min}(\pi, T)$  and  $\hat{G}_0^{\min}(\pi, T) = 0$  in the plane  $(\pi, T)$ .

To be concrete, let us specialize our results to the case that  $G(x; \pi, T)$  is an expansion in the order parameters of the free-energy of BaTiO<sub>3</sub>. Following Kim [53], we shall consider the following two possibilities, in which a possible dependence on the pressure  $\pi$  is ignored and CGS units are used:

$$\begin{aligned} c &= 7.4 \cdot (T - 110) \cdot 10^{-5} \\ B_0 &= 0, \\ A_0 &= 1.15 \cdot 10^{-12}, \\ A_1 &= (-0.99 - 1.15) \cdot 10^{-12}, \\ B_1 &= 0, \\ B_2 &= 0.249 \cdot 10^{-21}, \end{aligned} \quad (145)$$

$$\begin{aligned} c &= 7.4 \cdot (T - 110) \cdot 10^{-5}, \\ B_0 &= 0, \\ A_0 &= 12 \cdot 10^{-13}, \\ A_1 &= 4 \cdot 4.5 \cdot (T - 175) \cdot 10^{-15} - 12 \cdot 10^{-13}, \\ B_1 &= 24 \cdot 10^{-23}, \\ B_2 &= 30 \cdot 10^{-23}. \end{aligned} \quad (146)$$

Then, using the data specified in (145), for  $T > 119.97^\circ\text{C}$ , the free-energy takes on its absolute minimum at  $\Sigma_0$ ; thus only the disordered cubic phase [O<sub>h</sub>] is stable at these temperatures. At  $T = 119.97^\circ\text{C}$ , the function  $\hat{G}_1^{\min}(T)$  vanishes, so that the cubic and tetragonal phases coexist. For  $119.97^\circ\text{C} < T < 14.77$  the absolute minimum sits on  $\{C_{4v}\}$  and the tetragonal phase [C<sub>4v</sub>] is stable. At  $T = 14.77^\circ\text{C}$ , the absolute minimum shifts to  $\{C_{2v}\}$  and for  $14.77^\circ\text{C} < T < -87.49$  the stable phase is the orthorhombic one. At  $T = -87.49$  the absolute minimum shifts to  $\{C_{3v}\}$  and for  $T < -87.49$  the stable phase is the rhombohedral one.

These results, and the analogous ones obtained using the data specified in (146), of (146), are resumed in tables 6 and 7.

If the free energy is expanded as a sufficiently high degree polynomial in the order parameters  $x$ , and for a convenient choice of the coefficients as functions of  $T$ , all the phases represented by the isotropy type strata of the orbit space of  $O_h$  may become accessible (as stable phases) to the system at convenient temperatures. In particular, the sub-principal strata require at least a 8th degree polynomial, while the principal stratum requires at least a 12th degree polynomial.

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## 7 Tables and table captions

Table 1: Correspondence between classes of allowable solutions of the canonical equation (labelled by the degree  $d_1$ ) and finite coregular generating groups, for  $q = 2$ .

Group	$Z_2 \otimes Z_2$	$A_2, I_2(3)$	$B_2, I_2(4)$	$I_2(5)$	$G_2, I_2(6)$	$I_2(m)$
$d_1$	2	3	4	5	6	$m > 6$

Table 2: Correspondence between classes of fundamental allowable solutions of the canonical equation, degrees of the basic invariants and finite coregular generating groups, for  $q = 3$ .

Group	$I_2(m+1) \otimes Z_2$	$A_3, D_3$	$B_3$	$H_3$
$(d_1, d_2)$	$(m+1, 2)$	$(4, 3)$	$(6, 4)$	$(10, 6)$
Class	$II(m), m \in \mathbb{N}_*$	III.1	III.2	III.3

Table 3: Correspondence between classes of irreducible fundamental allowable solutions of the canonical equation, degrees of the basic invariants and finite coregular irreducible generating groups, for  $q = 4$ .

Group	$A_4$	$D_4$	$B_4$	$F_4$	$H_4$
$(d_1, d_2, d_3)$	$(5, 4, 3)$	$(6, 4, 4)$	$(8, 6, 4)$	$(12, 8, 6)$	$(30, 20, 12)$
Class	E1	E2	E3	E4	E5

Table 4: Correspondence between classes of reducible fundamental allowable solutions of the canonical equation, degrees of the basic invariants and finite coregular reducible generating groups, for  $q = 4$ .

Group	$I_2(j_1 + 1) \otimes I_2(j_2 + 1)$	$A_3 \otimes Z_2, D_3 \otimes Z_2$	$B_3 \otimes Z_2$	$H_3 \otimes Z_2$
$(d_1, d_2, d_3)$	$((j_1 + 1), (j_2 + 1), 2)$	$(4, 3, 2)$	$(6, 4, 2)$	$(10, 6, 2)$
Class	$A8(j_1, j_2), j_1 \geq j_2 \in \mathbb{N}_*$	$B4(1)$	$C6(1)$	$D4(1)$

Table 5: Isotropy type strata of the orbit space of the 3-dimensional representation of the group  $O_h$ .

Strata	Defining relations in $\mathbb{R}^q$	Typical points in $\mathbb{R}^n$
$\Sigma_0 = \{O_h\}$	$p_1 = p_2 = p_3 = 0$	$\bar{x}_1 = \bar{x}_2 = \bar{x}_3 = 0$
$\Sigma_1 = \{C_{4v}\}$	$f_1 = f_2 = 0 < p_3$	$\bar{x}_1 = 1, \bar{x}_2 = \bar{x}_3 = 0$
$\Sigma_3 = \{C_{3v}\}$	$f_3 = f_4 = 0 < p_3$	$\bar{x}_1 = \bar{x}_2 = \bar{x}_3 = 1$
$\Sigma_2 = \{C_{2v}\}$	$f_5 = f_6 = 0 < p_3$	$\bar{x}_1 = 0, \bar{x}_2 = \bar{x}_3 = 1$
$\Sigma_4 = \{C_s\}$	$f_8 = 0 < f_3, f_7, p_3$	$\bar{x}_1 = 1, \bar{x}_2 = \bar{x}_3 = 2$
$\Sigma_5 = \{C'_s\}$	$f_7 = 0 < f_1, f_5, p_3$	$\bar{x}_1 = 0, \bar{x}_2 = 1, \bar{x}_3 = 2$
$\Sigma_p = \{C_1\}$	$0 < f_7, f_8, p_3$	$\bar{x}_1 = 1, \bar{x}_2 = 2, \bar{x}_3 = 3$

Table 6: Stable phases of  $BaTiO_3$  at different temperatures with the first choice for the parameters involved in the definition of the free-energy.

Phase	Range of temperatures
$[O_h]$ =cubic	$T > 119.97^\circ\text{C}$
$[O_h], [C_{4v}]$	$T = T_{c_1} = 119.97^\circ\text{C}$
$[C_{4v}]$ =tetragonal	$119.97^\circ\text{C} > T > 14.77^\circ\text{C}$
$[C_{4v}], [C_{2v}]$	$T = T_{c_2} = 14.77^\circ\text{C}$
$[C_{2v}]$ =orthorhombic	$14.77^\circ\text{C} > T > -87.49^\circ\text{C}$
$[C_{2v}], [C_{3v}]$	$T = T_{c_3} = -87.49^\circ\text{C}$
$[C_{3v}]$ =rhombohedral	$-87.49^\circ\text{C} > T$

Table 7: Stable phases of BaTiO<sub>3</sub> at different temperatures with the second choice for the parameters involved in the definition of the free-energy.

Phase	Range of temperatures
[O <sub>h</sub> ] = cubic	$T > 115.40^\circ\text{C}$
[O <sub>h</sub> , [C <sub>4v</sub> ]	$T = T_{c_1} = 115.40^\circ\text{C}$
[C <sub>4v</sub> ] = tetragonal	$115.40^\circ\text{C} > T > -233.52^\circ\text{C}$
[C <sub>4v</sub> ], [C <sub>2v</sub> ]	$T = T_{c_2} = -233.52^\circ\text{C}$
[C <sub>2v</sub> ] = orthorhombic	$-233.52^\circ\text{C} > T$